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Minimization of dimension for functional differential equations and the thermodynamics of the classical one-dimensional fluid

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Abstract. The method of minimization of dimension for systems of first-order partial differential equations (PDEs) is extended analogously to systems of functional differential equations (FDEs). This method is applied to an exact first-order system of FDEs for the grand partition function of a one-dimensional classical fluid giving an alternative derivation of the pair potentials found by Baxter, for which exact thermodynamics can be obtained. These potentials satisfy a constant-coefficient ordinary differential equation (ODE). The method also gives the eigenvalue problem for the thermodynamics in these cases which is illustrated by deriving it explicitly for the simplest case, which is the exponential potential. The connection is derived between the finite system with external field to which the method applies and the infinite system without external field. This clarifies some points in Baxter's work and sheds some light on possible extensions of it.

1. Introduction

The interest in methods for obtaining 'exact' solutions for thermodynamics and structural properties for problems in classical equilibrium statistical mechanics of fluids defined by continuous potentials has continued until recent years. Apart from continuing interest in one-dimensional models with nearest neighbour potentials [1, 2] a new method applicable to the three-dimensional case has recently been proposed by Edgal [3] which makes use of nearest neighbour probability density functions (NNPDFs) which seem to have been largely ignored in the literature in favour of the n-body distribution functions. His scheme leads to an iterative process for calculating, simultaneously along the isotherms, the free-energy density and the NNPDFs which should converge to the exact solution. The most computationally demanding part of each cycle of the algorithm involves calculating an n-dimensional integral for each value of the density, where n is the number of particles which have a significant interaction with a given fixed particle which acts as a source of external field. Thus n may be 'a few tens' in practice while N the total number of particles in the system approaches infinity. He suggests that the integral may be evaluated by a Monte Carlo method and in principle exactness is only obtained when $n \to \infty$. The method is particularly appropriate for hard spheres and other systems with short ranged potentials and seems to be the natural extension to three dimensions of the exact analysis of one-dimensional systems with a finite number of nearest neighbours interacting. See for example Lieb and Mattis [4] for references to this earlier work.

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In this paper I present an alternative approach to the one-dimensional problem based on my previous work [5] in the light of a better understanding that I have obtained of the necessary theory of partial differential equations (PDEs) [6]. Hence I regard [5] as superseded by the present paper (except for mention of the beautiful result (4.6) for the nth functional derivative of the composition of two functionals). Unfortunately this work has developed in a way essentially independent of other recent contributors to the field. This may make it hard to understand but I ask the reader's allowance here because I believe the intrinsic interest in the methods used will justify the extra effort needed.

It has been shown earlier that the grand partition function (GPF) satisfies a functional difference–differential equation [7] and it can be written formally as an infinite system of first-order functional differential equations (FDEs) in many different ways [5]. I also showed [7] how one can formally treat a single first order FDE by the method of characteristics, treating functional derivatives in the same way as partial derivatives. Furthermore, I have recently shown [6] that there is a generalization of the theory of characteristics for systems of first order PDEs in n independent variables which in some cases gives an effectively complete reduction of dimension of the problem to dimension $r < n$ depending on the 'complexity' of the original system. In a typical case however, there will be no reduction of dimension so $r = n$. I give here a formal extension of this method to systems of FDEs and apply it to the first order system mentioned above. This eventually leads to Baxter's result [8] that the thermodynamics for any pair potential which satisfies an ordinary differential equation (ODE) of order $r - 1$ with constant coefficients can be obtained from an r-dimensional eigenvalue problem. The thermodynamics are obtained from a limiting process applied to the results for finite systems with external field which the method gives. I derive this explicitly for the simplest case $r = 2$ and show how the thermodynamics can be obtained which requires a discussion of the approach to the thermodynamic limit for a non-uniform system. This clarifies some important points which are not clear in Baxter's original paper [8].

This rederivation of Baxter's results is important because it is a means of checking the new mathematical methods developed here and because it presents Baxter's idea in a way in which generalization may be possible. Specifically, I believe that this could be done by using a formal extension to FDEs of an idea implicit in [6] namely repeated use of 'partial reduction to (one) dimension', solving the resulting equation and re-inserting the solution back into the original system so reducing the number of unknowns. This may lead to a wider class of potentials for which a finite-dimensional problem for the exact thermodynamics can be formulated. I am now trying to generalize this idea and then I hope to apply it to the above problem in a future publication.

The layout of this paper is as follows. In section 2 I introduce notation and derive necessary and sufficient conditions determining the GPF. Section 3 contains a formal argument, generalizing the arguments in [6], giving the procedure for minimization of dimension for any system of first-order FDEs. I then illustrate this general procedure in section 4 by applying it to the system obtained from the exact equations for the GPF. I also derive the explicit eigenvalue problem for the simplest case $r = 2$ i.e. the decaying exponential pair potential. In section 5 I summarize the results of the paper and explain how the work might be generalized to other classes of potentials.

In the appendix I discuss the approach to the thermodynamic limit for non-uniform systems in more general terms than are needed here, giving a short derivation of the asymptotic form for the GPF which holds for a slowly varying external field and shows the validity of local thermodynamics in this case. This result is implicit in the work of Percus [9] and is conceptually simpler than many other derivations [10–12] although the latter authors proceed from a more rigorous mathematical point of view.

2. Necessary and sufficient conditions for the GPF of the non-uniform system and the calculation of pressure

In the following I shall use square brackets to denote functionals because they are more commonly used than the braces I used earlier. I start with the GPF for the one-dimensional non-uniform fluid which can be written as

$$\Xi[L, z(x)] = \sum_{N=0}^{\infty} \frac{1}{N!} \int_0^L \mathrm{d}L_1 \int_0^L \mathrm{d}L_2 \ldots \int_0^L \mathrm{d}L_N \left(\prod_{i=1}^{N} z(L_i) \right) \mathrm{e}^{-\beta V_{\mathrm{IN}}} \quad (1)$$

which can be written in the equivalent form without the factor $1/N!$ and the integral restricted to the domain $0 \leqslant L_N \leqslant L_{N-1} \cdots \leqslant L_1 \leqslant L$. V_{IN} is the internal potential energy of the system i.e. the mutual interaction energy of all the particles. $V_{\mathrm{IN}} = \sum_{1 \leqslant i < j \leqslant N} \phi(L_i - L_j)$ when the potential energy is pairwise additive. With the exception of the appendix I shall be concerned entirely with this case. In (1) the system is of length L and $v(x) = \beta\phi(x)$ where ϕ is the pair potential and $\beta = 1/k_{\mathrm{B}}T$. If the external field is introduced into the problem of the statistical mechanics of a classical fluid the GPF provides a generating functional for the n-particle distribution functions. This was one of the original motivations for introducing it into the theory of liquids. It has been conveniently used in the form $z(x) = z\,\mathrm{e}^{-\beta V_E(x)}$ by Stell [13] (where z is the fugacity) in connection with cluster expansions of thermodynamic properties and correlation functions.

I have shown in [7, 14] that from Baxter's recurrence relation for the configuration integrals or directly by differentiation it follows that

$$\frac{\partial \Xi}{\partial L}[L, z(x)] = z(L)\,\Xi[L, z(x)\,\mathrm{e}^{-v(L-x)}]\,. \quad (2)$$

Introducing $G^*[L, z(x)] = \ln \Xi[L, z(x)]$ this can be written as

$$\frac{\partial G^*}{\partial L} = z(L) \exp\left(G^*[L, z(x)\,\mathrm{e}^{-v(L-x)}] - G^*[L, z(x)]\right)\,. \quad (3)$$

The form of (3) can be simplified, linearizing the argument function, by introducing

$$y(x) = \ln z(x) = \beta\mu + \frac{1}{2} \ln\left(\frac{2\pi m}{\beta h^2}\right) - \beta V_E(x) \quad (4)$$

where μ is the chemical potential, m is the mass of the particles and h is Planck's constant. The function $y(x)$ now plays the role of independent variable in the transformed equation which reads

$$\frac{\partial G}{\partial L} = \exp\{y(L) + G[L, y(x) - v(L-x)] - G[L, y(x)]\} \quad (5)$$

where the new functional G is defined by $G[L, y(x)] = G^*[L, \mathrm{e}^{y(x)}]$. Then in this notation the GPF becomes

$$\Xi = \mathrm{e}^G = \sum_{N=0}^{\infty} \frac{1}{N!} \int_0^L \mathrm{d}L_1 \ldots \int_0^L \mathrm{d}L_N \exp\left\{ \sum_{i=1}^{N} y(L_i) - \sum_{1 \leqslant i < j \leqslant N} v(L_i - L_j) \right\}. \quad (6)$$

Putting $L = 0$ leaves only the $N = 0$ term which is 1 so that

$$\Xi[0, z(x)] = 1 . \tag{7}$$

Equations (2) and (7) look like an initial-value problem with a unique solution. In fact this is true only if the L dependence of Ξ is only in the cut-off of the integrations i.e. $\Xi[L, z(x)]$ depends on $z(x)$ only in the range $x \in [0, L]$ and is otherwise independent of L. The general Maclaurin expansion of an analytical functional satisfying this condition is

$$\Xi[L, z(x)] = \sum_{N=0}^{\infty} \int_0^L dL_1 \int_0^{L_1} dL_2 \ldots \int_0^{L_{N-1}} dL_N \left(\prod_{i=1}^{N} z(L_i) \right) h_N(L_1, \ldots L_N) . \tag{8}$$

This is the expansion of any functional which depends on a single function $z(x)$ which is zero whenever $x < 0$ or $x > L$. The most general analytical functional of L and $z(x)$ in the interval $0 \leqslant x \leqslant L$ would have had the h_N factor as $h_N(L, L_1, L_2, \ldots L_N)$ with additional L dependence.

Substituting this form for Ξ into (2) gives an equation from which one can equate the kernel functions because it holds for all $z(x)$:

$$\left(\prod_{i=1}^{N} e^{-v(L-L_i)} \right) h_N(L_1, \ldots L_N) = h_{N+1}(L, L_1, \ldots L_N)$$

$$\text{for all} \quad L, L_1, \ldots L_N \quad \text{and} \quad N \geqslant 0 . \tag{9}$$

By writing down the equations explicitly for $N = 0, 1, 2 \ldots$ it is easy to conjecture then prove by induction that

$$h_N(L_1, L_2, \ldots L_N) = h_0 \exp\left(- \sum_{1 \leqslant i < j \leqslant N} v(L_i - L_j) \right) . \tag{10}$$

This may now be inserted into the RHS of (8) giving $h_0 \Xi[L, z(x)]$ which is the most general solution of (2) of the form (8) so the GPF is completely characterized by (2), (7) and (8).

For any non-uniform system the pressure at $x = L$ is

$$P = P_L = k_B T \frac{\partial \ln \Xi}{\partial L} \tag{11}$$

which depends only on β, μ and $V_E(x)$ for a fixed pair potential $\phi(x)$. Moreover βP is a function of only L,$y(x)$ and $v(x)$ so the chemical potential μ and $V_E(x)$ do not enter the problem separately but only in the combination $y(x)$. Since $v(x)$ is fixed in the whole argument, the determination of the functional $\beta P[L, y(x)]$ gives the thermodynamics of the non-uniform system for a given $v(x)$. The functional $\beta P[L, y(x)]$ degenerates to the function $\beta P(y(L))$ when the function y approaches a constant in a neighbourhood of $x = L$ sufficiently rapidly as $L \to \infty$. This is obvious on physical grounds but its derivation is given here in the appendix.

3. The method of minimization of dimension for systems of FDEs

In this section I describe the formal extension of the methods in [7] and [6] to systems of FDEs and in the next section I apply them to reproduce Baxter's basic results. I am writing this in detail here in the hope that these methods will find many applications outside the scope of this paper.

The essential idea is to look for the most advantageous sets of dependent and independent variables. For many cases no simplification is possible but for a single first-order FDE reduction to one dimension i.e. one independent variable is always possible [7] the result extending the classical calculation of solutions along characteristics for the PDE case. Here I am concerned with the generalization of this to systems of FDEs.

Let the system of FDEs be

$$F_k\left[y(x), L, \{u_i\}, \left\{\frac{\partial u_i}{\partial L}\right\}, \left\{\frac{\delta u_i}{\delta y(s)}\right\}\right] = 0 \qquad \text{for} \quad 1 \leqslant k \leqslant m \tag{12}$$

for the set of unknown functionals u_i for $1 \leqslant i \leqslant p$ of $L > 0$ and $y(x)$ for $0 \leqslant x < \infty$. The F_k are the functional analogues of the functions F_k I used earlier in [6] i.e. for given L and $y(x)$ the F_k depend on the u_i and their derivatives only at the same point $(L, y(x))$. Upon inserting a set of known functionals $u_i[L, y(x)]$ the F_k become dependent on L and $y(x)$ only. Here $0 \leqslant L < \infty$ and the function $y(x)$ is allowed to range over the space of all functions defined on the interval $0 \leqslant x < \infty$. The total derivatives are

$$\frac{\mathrm{d}F_k}{\mathrm{d}y(t)} = \frac{\delta F_k}{\delta y(t)} + \sum_{i=1}^{p}\left[\frac{\partial F_k}{\partial u_i}\frac{\delta u_i}{\delta y(t)} + \frac{\partial F_k}{\partial(\partial u_i/\partial L)}\frac{\delta}{\delta y(t)}\left(\frac{\partial u_i}{\partial L}\right) + \int_0^\infty \mathrm{d}s \frac{\delta F_k}{\delta(\delta u_i/\delta y(s))}\frac{\delta^2 u_i}{\delta y(s)\delta y(t)}\right] \tag{13}$$

and

$$\frac{\mathrm{d}F_k}{\mathrm{d}L} = \frac{\partial F_k}{\partial L} + \sum_{i=1}^{p}\left[\frac{\partial F_k}{\partial u_i}\frac{\partial u_i}{\partial L} + \frac{\partial F_k}{\partial(\partial u_i/\partial L)}\frac{\partial^2 u_i}{\partial L^2} + \int_0^\infty \mathrm{d}s \frac{\delta F_k}{\delta(\delta u_i/\delta y(s))}\frac{\partial}{\partial L}\left(\frac{\delta u_i}{\delta y(s)}\right)\right]. \tag{14}$$

Let $h\left[y(x), \boldsymbol{u}, \boldsymbol{F}, \mathrm{d}\boldsymbol{F}/\mathrm{d}L, \mathrm{d}\boldsymbol{F}/\mathrm{d}y(t)\right]$ be a functional which depends only on L, $y(x)$, $u_i(x)$, $\partial u_i/\partial L$ and $\partial u_i/\partial y(x)$ after expressions for $\boldsymbol{F}$ and its total derivatives have been inserted. In general such a functional without this condition will involve second derivatives of $\boldsymbol{u}$. This condition is that all the second derivatives vanish i.e.

$$\frac{\delta h}{\delta\left(\delta^2 u_i/\delta y(s)\delta y(t)\right)} = 0 \tag{15}$$

$$\frac{\delta h}{\delta[(\partial/\partial y(s))(\partial u_i/\partial L)]} = 0 \tag{16}$$

$$\frac{\partial h}{\partial(\partial^2 u_i/\partial L^2)} = 0. \tag{17}$$

Such a functional gives a new equation $F_{m+1} \overset{\text{def}}{=} h - h(\boldsymbol{F} = \boldsymbol{0}) = 0$ necessarily satisfied by the u_i which satisfy $F_1 = \cdots = F_m = 0$ already. The complete independent set of all

such functionals must be found at each stage and the whole process repeated until no new independent such functionals are obtained. The resulting system $F_i = 0$ for $1 \leqslant i \leqslant m$, where m now denotes the number of equations in the new augmented system, is said to be complete because there are no extra integrability conditions. This is analogous to the method I used in [6] for systems of nonlinear PDEs to obtain all the integrability conditions. This is a very difficult task to carry out in general. The method is probably most useful when the system (12) is already complete but not known to be so. The equations for h must then show that h has no dependence on the derivatives of F_k and this demonstrates the completeness.

The following argument shows that the conditions satisfied by h can be written in simpler form.

Equation (15) can be written as

$$\sum_{k=1}^{m} \int_0^\infty \mathrm{d}t' \frac{\delta h}{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t')\right)} \frac{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t')\right)}{\delta\left(\delta^2 u_i/\delta y(s)\delta y(t)\right)} = 0. \tag{18}$$

From (13) the last derivative is

$$\sum_{j=1}^{p} \int_0^\infty \mathrm{d}s' \frac{\delta F_k}{\delta\left(\delta u_j/\delta y(s')\right)} \delta_{ij}\delta(\{s', t'\}, \{s, t\}) \tag{19}$$

where the last factor $\delta(\{s', t'\}, \{s, t\})$ can be easily shown to be $\frac{1}{2}[\delta(s'-s)\delta(t'-t)+\delta(s'-t)\delta(t'-s)]$ provided the obvious extension of the definition of the functional derivative to functions of two or more variables is taken:

$$\frac{\delta F[f(x_1 \ldots x_N)]}{\delta f(x_1' \ldots x_N')} = \lim_{\epsilon \to 0} \frac{\partial}{\partial \epsilon} F[f(x_1 \ldots x_N) + \epsilon \prod_{i=1}^{N} \delta(x_i - x_i')] \tag{20}$$

and the symmetric function $\delta^2 u_i/(\delta y(s)\delta y(t))$ is replaced by the equivalent explicitly symmetrized form. Hence (15) can be written as

$$\sum_{k=1}^{m} \left[\frac{\delta h}{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t)\right)} \frac{\delta F_k}{\delta\left(\delta u_i/\delta y(s)\right)} + \frac{\delta h}{\delta\left(\mathrm{d}F_k/\mathrm{d}y(s)\right)} \frac{\delta F_k}{\delta\left(\delta u_i/\delta y(t)\right)} \right] = 0 \tag{21}$$

for $1 \leqslant i \leqslant p$; $0 \leqslant s, t < \infty$. Similarly from (16)

$$\int_0^\infty \mathrm{d}t \sum_{k=1}^{m} \frac{\delta h}{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t)\right)} \frac{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t)\right)}{\delta[(\delta/\delta y(s))(\partial u_i/\partial L)]} + \sum_{k=1}^{m} \frac{\partial h}{\partial\left(\mathrm{d}F_k/\mathrm{d}L\right)} \frac{\delta\left(\mathrm{d}F_k/\mathrm{d}L\right)}{\delta[(\delta/\delta y(s))(\partial u_i/\partial L)]} = 0 \tag{22}$$

and

$$\frac{\delta\left(\mathrm{d}F_k/\mathrm{d}y(t)\right)}{\delta[(\delta/\delta y(s))(\partial u_i/\partial L)]} = \frac{\partial F_k}{\partial\left(\partial u_i/\partial L\right)} \delta(t-s) \qquad \frac{\delta\left(\mathrm{d}F_k/\mathrm{d}L\right)}{\delta[(\delta/\delta y(s))(\partial u_i/\partial L)]} = \frac{\delta F_k}{\delta\left(\delta u_i/\delta y(s)\right)}$$

hence

$$\sum_{k=1}^{m} \left[\frac{\delta h}{\delta\left(\mathrm{d}F_k/\mathrm{d}y(s)\right)} \frac{\partial F_k}{\partial\left(\partial u_i/\partial L\right)} + \frac{\partial h}{\partial\left(\mathrm{d}F_k/\mathrm{d}L\right)} \frac{\delta F_k}{\delta\left(\delta u_i/\delta y(s)\right)} \right] = 0. \tag{23}$$

The finally from (17) it follows that

$$\sum_{k=1}^{m} \frac{\partial h}{\partial (\mathrm{d}F_k/\mathrm{d}L)} \frac{\partial F_k}{\partial (\partial u_i/\partial L)} = 0 \qquad \text{for} \quad 1 \leqslant i \leqslant p. \tag{24}$$

The next step in the general procedure is to look for linear combinations

$$\sum_{k=1}^{m} F_k h_{\alpha k}[L, y(x), u_1 \ldots u_p] = 0 \qquad \text{for} \quad 1 \leqslant \alpha \leqslant m' \tag{25}$$

of the equations such that if the new continuum of variables $z(x)$ and $z_1 \ldots z_r$ are introduced in place of $L, y(x)$ then each equation is independent of all derivatives with respect to $z(x)$. (L will be assumed to be varying over these r-dimensional subspaces of the function space so that one can assume $z_1 = L$ without loss of generality.) From the introduction of the new variables it follows that

$$\left.\frac{\delta u_j}{\delta y(s)}\right|_L = \sum_{i=2}^{r} \frac{\partial u_j}{\partial z_i} \left.\frac{\delta z_i}{\delta y(s)}\right|_L + \int_0^\infty \mathrm{d}t \frac{\delta u_j}{\delta z(t)} \left.\frac{\delta z(t)}{\delta y(s)}\right|_L \tag{26}$$

and

$$\left.\frac{\partial u_j}{\partial L}\right|_{y(s)} = \frac{\partial u_j}{\partial L} + \sum_{i=2}^{r} \frac{\partial u_j}{\partial z_i} \left.\frac{\partial z_i}{\partial L}\right|_{y(s)} + \int_0^\infty \mathrm{d}t \frac{\delta u_j}{\delta z(t)} \left.\frac{\partial z(t)}{\partial L}\right|_{y(s)}. \tag{27}$$

Applying this change of variables to (25) the reduction of dimension to r requires that

$$\frac{\delta}{\delta (\delta u_i/\delta z(t))} \sum_{k=1}^{m} F_k h_{\alpha k}[L, y(x), u] = 0. \tag{28}$$

Using the chain rule, this can be expressed in terms of derivatives with respect to the original variables thus

$$\frac{\partial}{\partial (\partial u_i/\partial L)} \sum_{k=1}^{m} F_k h_{\alpha k} \frac{\delta (\partial u_i/\partial L)}{\delta (\delta u_i/\delta z(t))} + \int_0^\infty \mathrm{d}s \frac{\delta (\delta u_i/\delta y(s))}{\delta (\delta u_i/\delta z(t))} \frac{\delta}{\delta (\delta u_i/\delta y(s))} \sum_{k=1}^{m} F_k h_{\alpha k} = 0. \tag{29}$$

Using the equations from the change of variables above, this can be simplified to

$$\sum_{k=1}^{m} h_{\alpha k} \frac{\partial F_k}{\partial (\partial u_i/\partial L)} \left.\frac{\partial z(t)}{\partial L}\right|_{y(s)} + \int_0^\infty \mathrm{d}s \frac{\delta z(t)}{\delta y(s)} \sum_{k=1}^{m} h_{\alpha k} \frac{\delta F_k}{\delta (\delta u_i/\delta y(s))} = 0 \tag{30}$$

which is a set of FDEs for $z(t)$ of the form

$$\frac{\partial z}{\partial L} f_0[L, y(x)] + \int_0^\infty \mathrm{d}s \frac{\delta z}{\delta y(s)} f[s; L, y(s)] = 0 \qquad \forall t \in [0, \infty) \tag{31}$$

for fixed i and α once u is known in terms of $L, y(x)$. Although the u are not known yet, these equations can still be used to help set up the conditions for determining the $z(t)$.

Regarding f as a vector field on the space of points $S = \{(L, y(x))\}$, with a separate 0 component and a continuum of components indexed by s, one can proceed analogously to the finite-dimensional situation by noting that the $z(t)$ must all be independent variables and are therefore independent solutions of (31) with f replaced by $f_{i\alpha}$ where

$$f_{i\alpha} = \left(\sum_{k=1}^{m} h_{\alpha k} \frac{\partial F_k}{\partial (\partial u_i / \partial L)}, \sum_{k=1}^{m} h_{\alpha k} \frac{\delta F_k}{\delta (\delta u_i / \delta y(s))} \right). \tag{32}$$

This suggests that the Lie algebra generated by the $f_{i\alpha}$ has orbits of dimension r i.e. the $f_{i\alpha}$ generate an r-dimensional manifold. To find the consequences of this, take the $f_{i\alpha}$ and take commutators and appropriate linear combinations to get a set of r commuting LI vector fields b_β in terms of which the $f_{i\alpha}$ can be expressed thus

$$f_{i\alpha} = \sum_{\beta=1}^{r} \lambda_{i\beta\alpha} b_\beta \tag{33}$$

i.e.

$$f_{i\alpha 0} = \sum_{\beta=1}^{r} \lambda_{i\beta\alpha} b_{\beta 0} \qquad \text{and} \quad f_{i\alpha}(s) = \sum_{\beta=1}^{r} \lambda_{i\beta\alpha} b_\beta(s) \tag{34}$$

where the $\lambda_{i\beta\alpha}$ are functions of $(L, y(x))$ for a given $u[L, y(x)]$. In each r-dimensional subspace of S in which the $z(t)$ are all fixed, the $z_1 \ldots z_r$ vary so the $\partial/\partial z_\beta$ must be interior to them and commuting so choose $\partial/\partial z_\beta = b_\beta$ or in components $\partial y(t)/\partial z_\beta = b_\beta(t)$ and $\partial L/\partial z_\beta = b_{\beta 0}$. From the original system (12) I have the equations

$$\frac{\mathrm{d}}{\mathrm{d}y(s)} \sum_{k=1}^{m} F_k h_{\alpha k} = 0$$

which together with (12) yield

$$\sum_{k=1}^{m} h_{\alpha k} \frac{\mathrm{d}F_k}{\mathrm{d}y(s)} = 0. \tag{35}$$

Substituting (13) into (35) the third term becomes (using (32) and (34))

$$\sum_{i=1}^{p} \sum_{\beta=1}^{r} \lambda_{i\beta\alpha} b_{\beta 0} \frac{\delta}{\delta y(s)} \left(\frac{\partial u_i}{\partial L} \right)$$

and the last term similarly becomes

$$\int_0^\infty \mathrm{d}t \sum_{i=1}^{p} \sum_{\beta=1}^{r} \lambda_{i\beta\alpha} b_\beta(t) \frac{\delta^2 u_i}{\delta y(s) \delta y(t)}.$$

From the chain rule

$$\frac{\partial}{\partial z_\beta} \left(\frac{\delta u_i}{\delta y(s)} \right) = \int_0^\infty \mathrm{d}t \frac{\delta}{\delta y(t)} \left(\frac{\delta u_i}{\delta y(s)} \right) \frac{\partial y(t)}{\partial z_\beta} + \frac{\partial}{\partial L} \left(\frac{\delta u_i}{\delta y(s)} \right) \frac{\partial L}{\partial z_\beta}. \tag{36}$$

Hence using $\partial/\partial z_\beta = b_\beta$ the equations become

$$\sum_{k=1}^{m} h_{\alpha k}\left(\frac{\delta F_k}{\delta y(s)} + \sum_{i=1}^{p}\frac{\partial F_k}{\partial u_i}\frac{\delta u_i}{\delta y(s)}\right) + \sum_{i=1}^{p}\sum_{\beta=1}^{r}\lambda_{i\beta\alpha}\frac{\partial}{\partial z_\beta}\left(\frac{\delta u_i}{\delta y(s)}\right) = 0 \tag{37}$$

for $1 \leqslant \alpha \leqslant m'$ and $0 \leqslant s < \infty$. A similar argument shows that, starting from

$$\frac{\mathrm{d}}{\mathrm{d}L}\sum_{k=1}^{m} F_k h_{\alpha k} = 0$$

and using (14), the chain rule, (32) and (34) the equations

$$\sum_{k=1}^{m} h_{\alpha k}\left(\frac{\partial F_k}{\partial L} + \sum_{i=1}^{p}\frac{\partial F_k}{\partial u_i}\frac{\partial u_i}{\partial L}\right) + \sum_{i=1}^{p}\sum_{\beta=1}^{r}\lambda_{i\beta\alpha}\frac{\partial}{\partial z_\beta}\left(\frac{\partial u_i}{\partial L}\right) = 0 \tag{38}$$

hold for $1 \leqslant \alpha \leqslant m'$. Also from the chain rule, and assuming that $L = z_1$,

$$\frac{\partial u_i}{\partial z_j} = \int_0^\infty \mathrm{d}s \frac{\delta u_i}{\delta y(s)}\frac{\partial y(s)}{\partial z_j} + \frac{\partial u_i}{\partial L}\frac{\partial L}{\partial z_j} = \int_0^\infty \mathrm{d}s \frac{\delta u_i}{\delta y(s)} b_j(s) + \frac{\partial u_i}{\partial L}\delta_{j1}\,. \tag{39}$$

Equations (37), (38) and (39) are the analogues of (55) and (56) of [6] and are the required equations involving only r independent variables as expected. The original independent variables $y(x)$ and the original unknowns $u_1 \ldots u_p$ and their first derivatives $\partial u_i/\partial L, \delta u_i/\delta y(s)$ should now be regarded as the new unknowns and $z_1 \ldots z_r$ as the new independent variables. In a systematic procedure for dealing with systems of the type (12), linear combinations α for which $r = 1$ should be sought first followed by those for which $r = 2$ etc. Of special interest are cases when the same set of vectors b_β will serve for a number of independent linear combinations of the system. If this number is equal to m the number of equations in the the system, the $h_{\alpha k}$ are completely arbitrary and the coefficients of them may be equated to zero to get the reduced r-dimensional system. This happens in this paper with $r \geqslant 2$ in the analysis in the next section of the equations defining the GPF.

4. The exact treatment of the equations for the GPF

To illustrate the technique of minimization of dimension of systems of FDEs described above it is necessary to express (5) as a first order system. In the RHS the difference term can be replaced by its functional Taylor expansion to N terms and later I will let $N \to \infty$. The result is

$$\frac{\partial G[L, y(x)]}{\partial L} = \exp\left(y(L) + \sum_{k=1}^{N}\frac{1}{k!}\int_0^\infty \mathrm{d}x_1 \ldots \int_0^\infty \mathrm{d}x_k \prod_{i=1}^{k}(-v(L - x_i))\frac{\delta^k G[L, y(x)]}{\delta y(x_1)\ldots\delta y(x_k)}\right) \tag{40}$$

which becomes formally exact as $N \to \infty$. Now the functionals $u_1 \ldots u_N$, each dependent on L and $y(x)$ are introduced by the following equations

$$u_1 = G \qquad \text{and} \qquad u_k = -\int_0^\infty \mathrm{d}x\, v(L - x)\frac{\delta u_{k-1}}{\delta y(x)} \qquad \text{for} \quad 2 \leqslant k \leqslant N\,. \tag{41}$$

Then in terms of the auxiliary variables $u_1 \ldots u_N$ equation (40) becomes first order:

$$\frac{\partial u_1}{\partial L} = \exp\left(y(L) + \sum_{i=1}^{N-1} \frac{u_{i+1}}{i!} - \frac{1}{N!}\int_0^\infty \mathrm{d}x\, v(L-x)\frac{\delta u_N}{\delta y(x)}\right) \stackrel{\text{def}}{=} E \tag{42}$$

hence in the notation of section 4 the resulting first order system of FDEs can be written as

$$F_1 = \frac{\partial u_1}{\partial L} - \exp\left(y(L) + \sum_{i=1}^{N-1} \frac{u_{i+1}}{i!} - \frac{1}{N!}\int_0^\infty \mathrm{d}x\, v(L-x)\frac{\delta u_N}{\delta y(x)}\right) = 0 \tag{43}$$

$$F_k = u_k + \int_0^\infty \mathrm{d}x\, v(L-x)\frac{\delta u_{k-1}}{\delta y(x)} = 0 \qquad \text{for} \quad 2 \leqslant k \leqslant N\,. \tag{44}$$

The first step of the procedure described above is to write down the derivatives of F_k WRT $\delta u_i/\delta y(x)$ and $\partial u_i/\partial L$ and obtain the equations for h to obtain the completion of the system (43) and (44):

$$\frac{\delta F_k}{\delta\,(\delta u_i/\delta y(s))} = (1-\delta_{k1})\delta_{i,k-1}v(L-s) + \delta_{k1}\frac{E}{N!}\delta_{i,N}v(L-s) \tag{45}$$

$$\frac{\partial F_k}{\partial\,(\partial u_i/\partial L)} = \delta_{k1}\delta_{i1}\,. \tag{46}$$

The equation (21) for h becomes

$$\sum_{k=1}^{N}\left[\frac{\delta h}{\delta\,(\mathrm{d}F_k/\mathrm{d}y(t))}\left((1-\delta_{k1})\delta_{i,k-1}v(L-s) + \delta_{k1}\frac{E}{N!}\delta_{iN}v(L-s)\right) + \text{same with } s \leftrightarrow t\right] = 0 \tag{47}$$

for $1 \leqslant i \leqslant N; 0 \leqslant s,t < \infty$. Doing the sums and specializing to the case $s = t$ and assuming $v \neq 0$ gives

$$\frac{\delta h}{\delta\,(\mathrm{d}F_k/\mathrm{d}y(s))} = 0 \qquad \text{for} \quad 1 \leqslant k \leqslant N\,. \tag{48}$$

From (23) for h,

$$\sum_{k=1}^{N}\left[\frac{\delta h}{\delta\,(\mathrm{d}F_k/\mathrm{d}y(s))}\delta_{k1}\delta_{i1} + \frac{\partial h}{\partial\,(\mathrm{d}F_k/\mathrm{d}L)}\left((1-\delta_{k1})\delta_{i,k-1}v(L-s) + \delta_{k1}\frac{E}{N!}\delta_{i,N}v(L-s)\right)\right] = 0\,. \tag{49}$$

For $i = 1$ it reduces to

$$\frac{\delta h}{\delta\,(\mathrm{d}F_1/\mathrm{d}y(s))} + \frac{\partial h}{\partial\,(\mathrm{d}F_2/\mathrm{d}L)}v(L-s) = 0 \tag{50}$$

so from above

$$\frac{\partial h}{\partial\,(\mathrm{d}F_2/\mathrm{d}L)} = 0\,. \tag{51}$$

The other cases are easy, combining to give

$$\frac{\partial h}{\partial\,(\mathrm{d}F_k/\mathrm{d}L)} = 0 \qquad \text{for} \quad 1 \leqslant k \leqslant N\,. \tag{52}$$

The final equation (24) for h is now trivial. Hence the conditions on h, (48) and (52), imply that h has no dependence on any of the first total derivatives of the F_k hence the system (43) and (44) is complete.

The next step is to write down the vector fields $f_{i\alpha}$ in (32) with separate 0 component $f_{i\alpha 0}$ and the continuum of components $f_{i\alpha}(s)$ for $0 \leqslant s < \infty$ which are defined at each point $(L, y(x))$ for $0 \leqslant L < \infty$ and $y(x)$ defined on $0 \leqslant x < \infty$. They are given by

$$f_{i\alpha 0} = \sum_{k=1}^{N} h_{\alpha k} \frac{\partial F_k}{\partial\,(\partial u_i/\partial L)} \qquad \text{and} \qquad f_{i\alpha}(s) = \sum_{k=1}^{N} h_{\alpha k} \frac{\delta F_k}{\delta\,(\delta u_i/\delta y(s))} \tag{53}$$

which for the above system simplify to

$$f_{i\alpha 0} = h_{\alpha 1}\delta_{i1} \qquad \text{and} \qquad f_{i\alpha}(s) = v(L-s)\left(h_{\alpha,i+1}(1-\delta_{i,N}) + h_{\alpha 1}\frac{E}{N!}\delta_{iN}\right) \tag{54}$$

for $1 \leqslant i \leqslant N$. Hence for each pair (i, α), $f_{i\alpha}$ is a linear combination of two vector fields which can be expressed in components as $(1, 0)$, $(0, v(L-s))$. Since this basis is independent of the choice of linear combination α, any linear combination of the original system is reduced in the same manifolds i.e the system is completely reduced to the number of dimensions r which is equal to the dimension of the manifolds generated by the two vectors. To determine this dimension a commuting basis in terms of which the $f_{i\alpha}$ can be expressed must be found. The differential operators associated with the vectors are

$$\tilde{b}_1 = \frac{\partial}{\partial L} \qquad \text{and} \qquad \tilde{b}_2 = \int_0^\infty \mathrm{d}s\, v(L-s)\frac{\delta}{\delta y(s)}\,. \tag{55}$$

Since $\tilde{b}_1$ is constant in these coordinates $L, y(x)$

$$[\tilde{b}_1, \tilde{b}_2] = \tilde{b}_1(\tilde{b}_2) = \int_0^\infty \mathrm{d}s\, v'(L-s)\frac{\delta}{\delta y(s)}\,. \tag{56}$$

Furthermore,

$$[\tilde{b}_1, [\tilde{b}_1, \ldots [\tilde{b}_1, \tilde{b}_2]\ldots] = \int_0^\infty \mathrm{d}s\, v^{(i)}(L-s)\frac{\delta}{\delta y(s)} \tag{57}$$

where $v^{(i)}$ is the ith derivative of $v(x)$ and $\tilde{b}_1$ appears i times. It also follows that the commutator of any pair of these operators is zero so that the set of operators

$$T_r = \left\{\tilde{b}_1; [\tilde{b}_1, [\tilde{b}_1, \ldots [\tilde{b}_1, \tilde{b}_2]\ldots] \qquad \text{where} \quad \tilde{b}_1 \text{ appears } i \text{ times for } i = 0, 1, 2\ldots\right\} \tag{58}$$

is closed under commutation i.e. forming a commutator of any pair of operators in T_r generates another one in T_r. Therefore r is the number of LI operators in T_r. Hence

$$\int_0^\infty \mathrm{d}s\, v^{(r-1)}(L-s)\frac{\delta}{\delta y(s)} = \sum_{i=0}^{r-2} B_i[L, y(x)] \int_0^\infty \mathrm{d}s\, v^{(i)}(L-s)\frac{\delta}{\delta y(s)} + A[L, y(x)]\frac{\partial}{\partial L} \tag{59}$$

for all s, L, $y(x)$. But B_i and A cannot depend on $y(x)$. Also equating the $\partial/\partial L$ components gives $A = 0$. Taking the s component gives

$$v^{(r-1)}(L-s) = \sum_{i=0}^{r-2} B_i(L) v^{(i)}(L-s) \qquad \text{for all } s \text{ and } L. \tag{60}$$

Finally B_i cannot depend on L so $v^{(r-1)}(x) = \sum_{i=0}^{r-2} B_i v^{(i)}(x)$ so for the r-dimensional case $v(x)$ must satisfy an ODE of order $r-1$ with constant coefficients. This agrees with the condition Baxter found for his equations to be finite-dimensional.

I will now derive these equations explicitly for the simplest case $r = 2$. Obviously

$$v(x) = D\,\mathrm{e}^{Bx} \tag{61}$$

where D is an arbitrary constant. Now a commuting basis $\boldsymbol{b}_1, \boldsymbol{b}_2$ for the vector space spanned by T_2 must be found. Let $\boldsymbol{b}_1 = \tilde{\boldsymbol{b}}_1$ and $\boldsymbol{b}_2 = \alpha\tilde{\boldsymbol{b}}_1 + \beta\tilde{\boldsymbol{b}}_2$ where α and β are dependent on L and $y(x)$. Then

$$[\tilde{\boldsymbol{b}}_1, \alpha\tilde{\boldsymbol{b}}_1 + \beta\tilde{\boldsymbol{b}}_2] = \beta[\tilde{\boldsymbol{b}}_1, \tilde{\boldsymbol{b}}_2] + \tilde{\boldsymbol{b}}_1(\beta)\cdot\tilde{\boldsymbol{b}}_2 + \tilde{\boldsymbol{b}}_1(\alpha)\cdot\tilde{\boldsymbol{b}}_1 = 0$$

or in components

$$\big(0, \beta v'(L-s)\big) + \left(0, \frac{\partial\beta}{\partial L} v(L-s)\right) + \left(\frac{\partial\alpha}{\partial L}, 0\right) = 0 \tag{62}$$

hence $\partial\alpha/\partial L = 0$ so $\alpha = \alpha[y(x)]$ and $\beta v'(L-s) + (\partial\beta/\partial L)v(L-s) = 0$ which is a ODE for β at fixed $y(x)$ when combined with (61). It has the general solution $\beta = \mathrm{e}^{-BL}c[y(x)]$. Hence the general solution for $\boldsymbol{b}_2$ is

$$\boldsymbol{b}_2 = \alpha[y(x)]\frac{\partial}{\partial L} + c[y(x)]\,\mathrm{e}^{-BL}\int_0^\infty \mathrm{d}s\, v(L-s)\frac{\delta}{\delta y(s)} \tag{63}$$

and the simplest choice giving LI $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, is

$$\boldsymbol{b}_2 = \mathrm{e}^{-BL}\int_0^\infty \mathrm{d}s\, v(L-s)\frac{\delta}{\delta y(s)} = D\int_0^\infty \mathrm{d}s\,\mathrm{e}^{-Bs}\frac{\delta}{\delta y(s)}. \tag{64}$$

The general theory can now be used to construct the corresponding equations in the two independent variables z_1 and z_2. To do this the coefficients $\lambda_{i\beta\alpha}$ have to be identified:

$$f_{i\alpha} = \sum_{\beta=1}^{2}\lambda_{i\beta\alpha}\boldsymbol{b}_\beta = \lambda_{i1\alpha}\frac{\partial}{\partial L} + \lambda_{i2\alpha}\,\mathrm{e}^{-BL}\int_0^\infty \mathrm{d}s\, v(L-s)\frac{\delta}{\delta y(s)} \tag{65}$$

so comparing with (54) shows that

$$\lambda_{i1\alpha} = h_{\alpha1}\delta_{i1} \qquad \text{and} \qquad \lambda_{i2\alpha} = \left(h_{\alpha,i+1}(1-\delta_{i,N}) + h_{\alpha1}\frac{E}{N!}\delta_{i,N}\right)\mathrm{e}^{BL}.$$

The derivatives of F_k WRT $y(s)$ taken at constant $\partial u_i/\partial L$ and $\delta u_i/\delta y(s)$ but allowing u_i to vary are

$$\frac{\delta F_k}{\delta y(s)} + \sum_{i=1}^{N}\frac{\partial F_k}{\partial u_i}\frac{\delta u_i}{\delta y(s)} = \begin{cases} -E\left(\delta(L-s) + \displaystyle\sum_{i=1}^{N-1}\frac{1}{i!}\frac{\delta u_{i+1}}{\delta y(s)}\right) & k = 1 \\ \dfrac{\delta u_k}{\delta y(s)} & 2 \leqslant k \leqslant N. \end{cases} \tag{66}$$

Introducing the new variables $z_1 = L$ and z_2 by the relations $\partial/\partial z_1 = b_1$, $\partial/\partial z_2 = b_2$ the derived equations (37) become

$$\sum_{k=1}^{N} h_{\alpha k}\begin{pmatrix} -E\left(\delta(L-s)+\sum_{i=1}^{N-1}(1/i!)\delta u_{i+1}/\delta y(s)\right) & k=1 \\ \delta u_k/\delta y(s) & 2\leqslant k\leqslant N\end{pmatrix}$$
$$+\sum_{i=1}^{N}\left[h_{\alpha 1}\delta_{i1}\frac{\partial}{\partial L}\left(\frac{\delta u_i}{\delta y(s)}\right)+\left(h_{\alpha,i+1}(1-\delta_{i,N})+h_{\alpha 1}\frac{E}{N!}\delta_{i,N}\right)\right.$$
$$\left.\times\, e^{BL}\frac{\partial}{\partial z_2}(\delta u_i/\delta y(s))\right]=0 \tag{67}$$

for $1\leqslant\alpha\leqslant N$; $0\leqslant s<\infty$. A similar set of equations derived from (38) can be written down but they will not be needed here. Since (67) hold within the same 2D manifolds for each value of α one can equate the coefficients of $h_{\alpha k}$. It turns out that only the cases $2\leqslant k\leqslant N$ will be required in which case one obtains

$$\frac{\delta u_k}{\delta y(s)}+e^{BL}\frac{\partial}{\partial z_2}\left(\frac{\delta u_{k-1}}{\delta y(s)}\right)=0$$

from which it follows that

$$\frac{\delta u_{i+1}}{\delta y(s)}=\left(-e^{BL}\frac{\partial}{\partial z_2}\right)^{i}\frac{\delta u_1}{\delta y(s)}\qquad\text{for}\quad 0\leqslant i\leqslant N-1\,. \tag{68}$$

From the original system of FDEs (44) this leads to the result that

$$u_{i+1}=-\int_0^\infty dx\, v(L-x)\left(-e^{BL}\frac{\partial}{\partial z_2}\right)^{i-1}\frac{\delta u_1}{\delta y(x)}\qquad\text{for}\quad 1\leqslant i\leqslant N-1\,. \tag{69}$$

Using these last two results, and the identity

$$\frac{\partial}{\partial z_2}=e^{-BL}\int_0^\infty ds\, v(L-s)\frac{\delta}{\delta y(s)}$$

from (42) the exponential term E in (43) simplifies giving

$$E=\exp\left[y(L)+\sum_{i=1}^{N}\frac{1}{i!}\left(-e^{BL}\frac{\partial}{\partial z_2}\right)^{i}u_1\right]. \tag{70}$$

Letting $N\to\infty$, this gives formally from (43)

$$\frac{\partial u_1}{\partial L}=\exp[y_{z_2}(L)+u_1(L,z_2-e^{BL})-u_1(L,z_2)] \tag{71}$$

where $y_{z_2}(x)$ is given by the equation

$$\frac{\partial y(x)}{\partial z_2}=\int_0^\infty ds\frac{\delta y(x)}{\delta y(s)}v(L-s)\,e^{-BL}=v(L-x)\,e^{-BL} \tag{72}$$

with solution $y_{z_2}(x) = z_2 v(L-x)\,e^{-BL} + y_0(x)$. Hence, substituting for $y_{z_2}(x)$ and $v(x)$ from (61) and remembering that $u_1 = \ln \Xi$ one obtains from (71)

$$\frac{\partial}{\partial L}\Xi[L, Dz_2\,e^{-Bx} + y_0(x)] = e^{(z_2 D\,e^{-BL} + y_0(L))}\,\Xi[L, z_2 D\,e^{-Bx} - D\,e^{B(L-x)} + y_0(x)] \tag{73}$$

which is easily seen to be equivalent to the exact equation (3.1) of [7] which can be written as

$$\frac{\partial}{\partial L}\Xi[L, y(x)] = e^{y(L)}\,\Xi[L, y(x) - v(L-x)] \tag{74}$$

where the substitutions $y(x) = y_0(x) + Dz_2\,e^{-Bx}$ and $v(L-x) = D\,e^{B(L-x)}$ have been made which make this equation effectively two-dimensional.

To show this explicitly define

$$\Xi^*(L, z_2) = \Xi[L, Dz_2\,e^{-Bx} + y_0(x)] \tag{75}$$

for fixed $y_0(x)$, D, and B. Then it follows that

$$\left.\frac{\partial \Xi^*}{\partial L}\right|_{z_2}(L, z_2) = \exp\left[z_2 D\,e^{-BL} + y_0(L)\right]\Xi^*\left(L, z_2 - e^{BL}\right). \tag{76}$$

Now introduce the new variable $z_3 = z_2\,e^{-BL}$ to transform (76) to variables separable type, then

$$\left.\frac{\partial}{\partial L}\right|_{z_2} = \left.\frac{\partial}{\partial L}\right|_{z_3} - Bz_3\frac{\partial}{\partial z_3}.$$

Let $\Xi(L, z_3) = \Xi^*(L, z_2)$ then (76) can be written in terms of $\Xi(L, z_3)$ as follows:

$$\frac{\partial \Xi}{\partial L} - Bz_3\frac{\partial \Xi}{\partial z_3} = \exp\left[Dz_3 + y_0(L)\right]\Xi(L, z_3 - 1). \tag{77}$$

If y_0 is a constant function one can look for solutions $\Xi(L, z_3)$ in the form $f_1(L)f_2(z_3)$. Inserting this into (77) and dividing by $f_1(L)f_2(z_3)$ according to the usual method gives

$$\frac{f_1'(L)}{f_1(L)} - Bz_3\frac{f_2'(z_3)}{f_2(z_3)} = \exp(Dz_3 + y_0)\frac{f_2(z_3 - 1)}{f_2(z_3)}. \tag{78}$$

Introducing $\gamma = f_1'(L)/f_1(L)$ which from (78) must be a constant, then $f_1(L) = c_\gamma\,e^{\gamma L}$ and

$$\gamma f_2(z_3) = \exp(Dz_3 + y_0) f_2(z_3 - 1) + Bz_3 f_2'(z_3). \tag{79}$$

Denote the solutions of (79) by $f_{2\gamma}(z_3)$ (with an arbitrary normalization constant) then a solution of (77) is $\Xi(L, z_3) = c_\gamma\,e^{\gamma L} f_{2\gamma}(z_3)$ and hence because (77) is a linear equation the solutions can be superposed giving the general solution of (73) in the form

$$\Xi(L, z_3) = \sum_\gamma c_\gamma\,e^{\gamma L} f_{2\gamma}(z_3). \tag{80}$$

The constants c_γ must be chosen so that

$$1 = \Xi(0, z_3) = \sum_\gamma c_\gamma f_{2\gamma}(z_3)\,. \tag{81}$$

This determines all the c_γ and hence gives the unique solution for Ξ for the system of length L with $y(x) = y_0 + Dz_3\,e^{B(L-x)}$.

In order that $k_BTv(x)$ is a physically acceptable pair potential it is necessary that $B < 0$. There is therefore an external field parameter $y(x)$ which increases exponentially with x and so $(1/\beta)(\partial \ln \Xi/\partial L)|y$ gives the pressure at $x = L$ in the non-uniform system but it cannot be equated with the thermodynamic pressure for the system given by $v(x)$ and $y(x) =$ constant which is what I wish to obtain. The way round this is to calculate the pressure at $x = 0$ instead. This can be shown to be given by $(1/\beta)(\partial \ln \Xi/\partial L)|_{\tilde{y}}$ where $\tilde{y}(x) = y(L-x)$ by the change of variables $x \to L-x$ applied to the particles of the system. In this case $\tilde{y}(x) = y_0(L-x)+Dz_2\,e^{-BL}\cdot e^{Bx}$ which can be made to be a fixed function of x by choosing $y_0 =$ constant and $z_2\,e^{-BL} = z_3$ also constant. Also $y(x) = y_0 + Dz_3\,e^{BL}\,e^{-Bx}$ is a function which approaches y_0 as $L \to \infty$ keeping z_3 fixed. Hence in this limit the pressure at $x = 0$ given by $(1/\beta)(\partial \ln \Xi/\partial L)|_{z_3}$ will approach $P(y_0)$, the thermodynamic pressure evaluated for a uniform system with $\ln z = y_0$ as shown in the appendix.

This justifies the choice of z_3 as new variable and

$$\beta P(y_0) = \lim_{L\to\infty} \frac{\partial \ln \Xi}{\partial L}\bigg|_{z_3} = \lim_{L\to\infty} \frac{\sum_\gamma c_\gamma \gamma\, e^{\gamma L} f_{2\gamma}(z_3)}{\sum_\gamma c_\gamma\, e^{\gamma L} f_{2\gamma}(z_3)} = \gamma_0 \tag{82}$$

which is the eigenvalue γ_0 of

$$\gamma f_2(z_3) = \exp(Dz_3 + y_0) f_2(z_3 - 1) + Bz_3 f_2'(z_3) \tag{83}$$

with the largest real part. This follows because it is the term corresponding to the largest eigenvalue which dominates the numerator and denominator as $L \to \infty$. It is easily seen that (83) may determine a piecewise analytic function on successive intervals of unit length but there is also the condition that f_2 is analytic. This follows from Ξ^* being analytic WRT z_2 (which controls the strength of the external field in (75)). This condition is referred to as the eigenvalue condition because it requires γ to be an eigenvalue of the operator applied to f_2 in the RHS of (83). I should point out that the whole problem has now been reduced to a 3-parameter (D, B, y_0) eigenvalue problem in one dimension but because one of the parameters (B) has dimensions L^{-1} which is related to the length of the system this parameter can be removed by a change of variables.

Using (61), with the GPF for the uniform system expressed in the form $\Xi(z, L, D, B)$ the change of variable $BL_i = \bar{L}_i$ shows that the GPF can also be written as $\Xi(z/B, BL, D, 1)$. Using the formula $\beta P = \lim_{L\to\infty} \ln \Xi/L$ gives $\gamma_0(z, D, B) = \gamma_0(z/B, D, 1) \times B$. This also follows from (83) by dividing by B leading to the 2-parameter eigenvalue problem for $\gamma^* = \gamma/B$:

$$\gamma^* f(x) = t\,e^{Dx} f(x-1) + xf'(x) \tag{84}$$

where $t = z/B$ and the eigenvalue with smallest real part is γ_0/B because $B < 0$; the eigenvalue condition is that f is analytic.

5. Summary and outlook

The method of minimization of dimension for systems of PDEs [6] has been formally extended to systems of FDEs and the method has been successfully applied to a functional Taylor expansion of the general equation satisfied by the GPF of a one-dimensional classical fluid which is really an identity derived by differentiation. The method reproduces Baxter's [8] solvable cases for the thermodynamics and correlation functions when the system of FDEs is simultaneously reducible to lower dimension i.e. when the pair potential satisfies a constant coefficient ODE. I have illustrated this general result by rederiving the explicit eigenvalue problem for the simplest of these cases namely when the pair potential is of decaying exponential form clarifying the role of the external field and the approach to the thermodynamic limit.

Furthermore, I have recently found a simple example of a system of PDEs which may be completely analytically solved by repeated 'partial minimization of dimension' i.e. reduction of dimension of a linear combination of the original system to one and re-inserting the analytic solution of the equation obtained so reducing the number of unknowns by one at each step. The system was about the simplest possible i.e. a constant coefficient linear first order system with three equations, three unknowns in three dimensions which does not involve the undifferentiated unknowns. It seems that in general the system of PDEs must be of a very special type (though not necessarily linear) to be amenable to this simple idea based on my earlier [6] work but a formal extension of this idea to FDEs must be possible and this might extend the class of potentials for which the thermodynamics can be obtained exactly or provide the framework for a proof that this class cannot be extended (for the finite potential single component case). I hope to report on this shortly.

Finally I would like to make a remark on the possible extension of the methods to real three-dimensional systems. It has always been my long term aim to obtain practical methods to exactly solve problems of physical interest in this field but I have always believed that the mathematical developments needed would be discovered by first trying to solve one-dimensional problems and then trying to generalize them. In this context I believe that an important idea is contained in the work of Edgal [3] cited in the introduction, namely the ordering of the particle coordinates which makes his formalism for the three-dimensional case look in places like that appropriate to a one-dimensional system. Since the supposed absence of such an ordering relation in three dimensions was once thought to be the reason for the non-generalizability of the methods in one dimension to three dimensions I think some generalizations may be possible to three-dimensional systems using this idea.

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Appendix. Thermodynamics and the finite non-uniform system

I shall start by giving a derivation of an important identity used by Lebowitz and Penrose [15] to obtain rigorously the thermodynamics of systems with an additional weak long ranged Kac potential.

Consider an expression involving the multiple integration

$$\int_0^L \mathrm{d}L_1 \ldots \int_0^L \mathrm{d}L_N .$$

I want to equate this to an expression involving integrations over the subintervals Ω_i for $1 \leqslant i \leqslant M$ which form a partition of the interval $[0, L]$. Since one can write $\int_0^L \mathrm{d}L_1 = \sum_{i=1}^M \int_{\Omega_i} \mathrm{d}L_1$ it follows that

$$\int_0^L \mathrm{d}L_1 \cdots \int_0^L \mathrm{d}L_N = \sum_{i_1=1}^M \cdots \sum_{i_N=1}^M \int_{\Omega_{i_1}} \mathrm{d}L_1 \cdots \int_{\Omega_{i_N}} \mathrm{d}L_N .$$

From the sequence $(i_1, i_2 \ldots i_N)$ the set of 'occupation numbers' $n_1, n_2 \ldots n_M$ can be found, n_j being the number of times j appears in the sequence $(i_1 \ldots i_N)$. L_i represents the coordinate of the ith particle in the system and n_j is the number of particles in the subsystem Ω_j. Each sequence $(n_1 \ldots n_M)$ can be obtained from many distinct sequences $(i_1 \ldots i_N)$, their number being obtained from the following argument from probability theory. This is equivalent to asking for the number of ways in which M boxes can be filled with a total of N distinguishable objects with n_j objects in box j for $1 \leqslant j \leqslant M$. Box 1 can be filled in $N!/((N-n_1)!n_1!)$ distinct ways. For each of these, box 2 may be filled in $(N-n_1)!/((N-n_1-n_2)!n_2!)$ distinct ways, etc. Hence the total number of ways of filling all the boxes is the product of these cancelling down to $N!/(n_1!n_2! \cdots n_M!)$. Returning to the integrals one obtains the transformation

$$\int_0^L \mathrm{d}L_1 \cdots \int_0^L \mathrm{d}L_N = \sum_{\substack{(n_1 \ldots n_M) \\ \sum_{i=1}^M n_i = N}} \frac{N!}{n_1!n_2! \cdots n_M!} \int_{\Omega_{i_1}} \mathrm{d}L_1 \cdots \int_{\Omega_{i_N}} \mathrm{d}L_N .$$

Hence regrouping the integrals and renaming the integration variables on Ω_j as $L_j^{(1)} \ldots L_j^{(n_j)}$ it can be written as

$$\int_0^L \mathrm{d}L_1 \cdots \int_0^L \mathrm{d}L_N = N! \sum_{\substack{(n_1 \ldots n_M) \\ \sum_{i=1}^M n_i = N}} \frac{1}{n_1!} \int_{\Omega_1} \mathrm{d}L_1^{(1)} \cdots \int_{\Omega_1} \mathrm{d}L_1^{(n_1)} \cdots \frac{1}{n_M!} \int_{\Omega_M} \mathrm{d}L_M^{(1)} \cdots \int_{\Omega_M} \mathrm{d}L_M^{(n_M)} .$$

If for all $N \geqslant 0$, f_N is a symmetric function of its N arguments summing over N removes the restriction and interchanging the sum and products gives

$$\sum_{N=0}^{\infty} \frac{1}{N!} \int_0^L \mathrm{d}L_1 \cdots \int_0^L \mathrm{d}L_N f_N(L_1 \cdots L_N) = \prod_{j=1}^M \left(\sum_{n_j=0}^{\infty} \frac{1}{n_j!} \int_{\Omega_j} \mathrm{d}L_j^{(1)} \cdots \int_{\Omega_j} \mathrm{d}L_j^{(n_j)} \right)$$
$$\times f_N \left(L_1^{(1)} \ldots L_1^{(n_1)}, L_2^{(1)} \ldots L_2^{(n_2)}, \ldots L_M^{(1)} \ldots L_M^{(n_M)} \right) \qquad \text{(A1)}$$

the symmetry of f_N allowing its arguments to be rearranged. This is the basic identity that was needed. In the right hand member of (A1) the product over j indicates the application of M commuting integral operators to f_N. The $n_j = 0$ terms represent 0 integrations which is by convention the identity operator 1. Putting

$$f_N(L_1 \ldots L_N) = \mathrm{e}^{-\beta V_{\mathrm{IN}}(L_1 \ldots L_N)} \prod_{j=1}^N z(L_i)$$

where V_{IN} is the internal potential energy of the N particle system (not necessarily pairwise additive) it becomes the GPF. I can set $M = 2$ and write $V_{IN} = \sum_{j=1}^{2} V_{I,n_j} + I_{\Omega_1,\Omega_2}$ where I_{Ω_1,Ω_2} is the potential energy of interaction between the subsystems Ω_1 and Ω_2. Hence from (A1)

$$\sum_{N=0}^{\infty} \frac{1}{N!} \int_0^L \mathrm{d}L_1 \ldots \int_0^L \mathrm{d}L_N \, \mathrm{e}^{-\beta V_{IN}(L_1 \ldots L_N)} \prod_{i=1}^{N} z(L_i) = \sum_{n_1=0}^{\infty} \frac{1}{n_1!} \int_{\Omega_1} \mathrm{d}L_1^{(1)} \ldots \int_{\Omega_1} \mathrm{d}L_1^{(n_1)}$$

$$\times \mathrm{e}^{-\beta V_{In_1}} \prod_{i=1}^{n_1} z(L_1^{(i)}) \Bigg(\sum_{n_2=0}^{\infty} \frac{1}{n_2!} \int_{\Omega_2} \mathrm{d}L_2^{(1)} \ldots$$

$$\ldots \int_{\Omega_2} \mathrm{d}L_2^{(n_2)} \, \mathrm{e}^{-\beta V_{In_2}} \, \mathrm{e}^{-\beta I_{\Omega_1,\Omega_2}} \prod_{i=1}^{n_2} z(L_2^{(i)}) \Bigg) . \tag{A2}$$

Dividing this by the corresponding expression with $I_{\Omega_1,\Omega_2} = 0$ following gives the grand canonical average $\langle \mathrm{e}^{-\beta I_{\Omega_1,\Omega_2}} \rangle$ of $\mathrm{e}^{-\beta I_{\Omega_1,\Omega_2}}$ with the two systems Ω_1 and Ω_2 adjacent but non-interacting i.e. the joint probability distribution of configurations of the system $\Omega_1 + \Omega_2$ is the product of the distributions of the configurations of the subsystems Ω_1 and Ω_2. With $I_{\Omega_1\Omega_2} = 0$ (A2) gives

$$\Xi^*[z(x), 0 \leqslant x \leqslant L] = \Xi[z(x), x \in \Omega_1] \times \Xi[z(x), x \in \Omega_2] = \Xi_1 \Xi_2 \tag{A3}$$

where in Ξ^* all contributions to the potential arising from sets of particles with some particles in each subsystem are zero. Equation (A2) can be written as

$$\frac{\ln \Xi - \ln \Xi_1}{|\Omega_2|} = \frac{\ln \Xi_2}{|\Omega_2|} + \frac{\ln \langle \mathrm{e}^{-\beta I_{\Omega_1\Omega_2}} \rangle}{|\Omega_2|} \tag{A4}$$

where $|\Omega_i|$ is the length of subsystem i. In the following I shall be concerned with the asymptotic analysis of Ξ obtained by requiring $y(x)$ to vary with L in a specified way as the limit $L \to \infty$ is taken. A simple way to formulate this is to specify a function $\tilde{y}$ which varies over the space of points $(L, y(x))$ and which is required to be fixed for the limiting process. In order to include the case $\tilde{y}(x) = y(x/L)$, the macroscopic external field, I define

$$\tilde{y}(t) = K[t, L, y(x)] . \tag{A5}$$

Suppose that K and $\tilde{y}$ are such that there exists a function $\Omega_2(L)$ such that $L/\Omega_2, \Omega_2 \to \infty$ as $L \to \infty$ and $y(x)$ approaches a finite constant value on $\Omega_2 = [L - |\Omega_2|, L]$. Under these conditions the density is going to become constant on Ω_2 as L increases and $\langle \mathrm{e}^{-\beta I_{\Omega_1,\Omega_2}} \rangle$ can be assumed to be independent of the sizes of the subsystems provided they are large compared with the range of the pair interaction $v(x)$. Then from (A4), independently of the way that $L/\Omega_2, \Omega_2 \to \infty$,

$$\lim_{L/\Omega_2,\Omega_2 \to \infty} \frac{\ln \Xi - \ln \Xi_1}{|\Omega_2|} = \lim_{|\Omega_2| \to \infty} \frac{\ln \Xi_2}{|\Omega_2|} . \tag{A6}$$

To express (A4) fully requires three independent variables for Ξ namely

(1) L determining the relationship between $\tilde{y}$ and y,

(2) $\tilde{y}$ the macroscopic external field parameter determining y the external field parameter,
(3) s between 0 and 1 determining the fraction of L which is the length of the system,

i.e. $\Xi[L, \tilde{y}, s]$ is defined as follows: from L and $\tilde{y}$ obtain y from the inverse of (A5) and the length of the system is sL from which Ξ is defined by (1). Thus

$$\frac{\ln \Xi - \ln \Xi_1}{|\Omega_2|} = \frac{\ln \Xi[L, \tilde{y}, 1] - \ln \Xi[L, \tilde{y}, 1 - |\Omega_2|/L]}{|\Omega_2|/L} \times \frac{1}{L}. \tag{A7}$$

In the limiting process defined above $L/|\Omega_2| \to \infty$ hence the first quotient on the RHS can be replaced by its limiting value $(\partial/\partial s) \ln \Xi[L, \tilde{y}, s]|_{s=1}$ under the limit. Finally the limit can be represented by $L \to \infty$ because the only remaining free variable $\tilde{y}$ is a fixed function:

$$\lim_{L/\Omega_2, \Omega_2 \to \infty} \frac{\ln \Xi - \ln \Xi_1}{|\Omega_2|} = \lim_{L \to \infty} \left(\frac{\partial}{\partial s} \ln \Xi[L, \tilde{y}, s] \bigg|_{s=1} \times \frac{1}{L} \right). \tag{A8}$$

From (11) and changing to the above notation

$$\beta P_L = \frac{\partial \ln \Xi}{\partial L}\bigg|_y = \frac{\partial}{\partial (sL)}\bigg|_{L, \tilde{y}} \ln \Xi[L, \tilde{y}, s]\bigg|_{s=1} = \frac{\partial}{\partial s} \ln \Xi[L, \tilde{y}, s]\bigg|_{s=1} \times \frac{1}{L} \tag{A9}$$

where P_L is the pressure at $x = L$ in the system given by $y(x)$ for $0 \leqslant x \leqslant L$. Combining (A9), (A8) and (A6) shows that

$$\lim_{L \to \infty} \beta P_L \bigg|_{\tilde{y}} = \lim_{\Omega_2 \to \infty} \frac{\ln \Xi_2}{|\Omega_2|}. \tag{A10}$$

The LHS is the limiting value of βP at $x = L$ which is shown to be equal to the usual expression for the thermodynamic pressure $\lim_{L \to \infty} \ln \Xi / L$ and the result, by the RHS, depends only on the unique limit $y = \lim_{L \to \infty} y(x)|_{\tilde{y}} x \in \Omega_2$ so the relationship between the pressure P and the external field y at the same point $x = L$ approaches a limit, independent of K provided K satisfies the condition above. It is the same as the thermodynamic relationship $P(y)$.

By using the identity (A1) in a different way it is possible to give a short elegant derivation of the asymptotic form of the GPF discussed rigorously in [11] and which is intimately related to local thermodynamics [16, 9]. From (A1) with the same f_N, arbitrary M and writing

$$V_{\text{IN}} = \sum_{j=1}^{M} V_{In_j} + I_M$$

where I_M is the interaction energy between the M subsystems Ω_j it follows by a similar argument to the derivation of (A4) that

$$\Xi[y(x); 0 \leqslant x \leqslant L] = \langle \mathrm{e}^{-\beta I_M} \rangle_{\text{subsystems independent}} \times \prod_{j=1}^{M} \Xi[y(x); x \in \Omega_j]. \tag{A11}$$

The subscript is intended to indicate that the grand canonical average is taken with the interaction terms I_M removed from the total potential energy. This can be written as

$$\frac{\ln \Xi[y(x); 0 \leqslant x \leqslant L]}{L} = \frac{1}{M} \sum_{j=1}^{M} \frac{\ln \Xi[y(x); x \in \Omega_j]}{L/M} + \frac{\ln \langle \mathrm{e}^{-\beta I_M} \rangle}{L}. \tag{A12}$$

I now suppose that $y(x) = y^*(x/L)$ so that the whole system is in a slowly varying external potential. As before a physically reasonable assumption will be made namely that I_M is roughly a sum of contributions from neighbouring subsystems so that $\langle I_M \rangle$ and $\langle e^{-\beta I_M} \rangle$ are of order M. Hence letting $M, L/M \to \infty$ keeping y^* fixed and assuming that the thermodynamic limit exists for each subsystem

$$\lim_{L\to\infty} \frac{\ln \Xi[y^*(x/L); 0 \leqslant x \leqslant L]}{L} = \int_0^1 ds \beta P(y^*(s))$$

$$\text{or} \qquad \ln \Xi \sim L \int_0^1 ds\, \beta P(y^*(s)) + o(L)\,. \tag{A13}$$

There is however a non-local correction [16] to $\partial n/\partial \mu$ involving the total correlation function of Ornstein and Zernike. This shows the limitations of this result and will give significant corrections in the $o(L)$ term when $y(x)$ varies significantly on the length scale of the total correlation function. In particular these corrections will be significant for uniform systems when L is not very large compared with the range of the correlations as occurs in the neighbourhood of the critical point [17]. The same considerations must apply to (A10) which is consistent with the expectation that numerical methods based on this formalism for the calculation of $P(y)$ will fail in a neighbourhood of a critical point, should one be found.

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