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Optimal variational approximations to renormalisation group transformations I. Theory

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Abstract. A variational approximation to a renormalisation group transformation involves a sequential selection of the variational parameters. We show that this problem is equivalent to a discrete-time optimal control problem. The application of ideas and techniques from control theory, such as dynamic programming and the Pontryagin maximum principle, are discussed, together with some of the basic problems posed by variational approximations. In particular, the Kadanoff criterion for determining the 'best' approximation to the fixed point is re-derived in a way which illustrates the basic underlying assumptions. An alternative criterion, which avoids the problems and inconsistencies of the Kadanoff criterion, is advanced.

1. Introduction

The possibility of developing variational approximations to real-space renormalisation group transformations was originally suggested by Kadanoff (1975). The basic idea behind Kadanoff's approach lies in the use of approximate recursion relations, which yield either an upper or lower bound to the exact free energy. An optimum bound can then be obtained by varying any free parameters in the basic renormalisation group transformation. Whilst there is, of course, no guarantee that any such bound need be particularly close to the exact free energy, this procedure does give an objective criterion for choosing a 'best' transformation from a class of transformations treated within a specified approximation.

In practice, Kadanoff (1975) obtained remarkably accurate estimates for the critical exponents of Ising systems on d-dimensional hypercubic lattices ($d = 2, 3, 4$) from a simple optimized lower bound approximation—the so-called one hypercube approximation. Subsequently, Kadanoff *et al* (1976) extended this calculation to compute the specific heat and spontaneous magnetisation of the two-dimensional Ising model and found excellent agreement with the known analytic results. In addition, they applied the approximation to the transformation of Bell and Wilson (1974) of a generalised Gaussian model (continuous spin model with s^4-weight factor) in $4-\epsilon$ dimensions. To first order in ϵ, the optimum transformation gave critical exponents in agreement with those obtained from conventional ϵ-expansions (Wilson and Fisher 1972, Wilson 1972). More recently, the Kadanoff lower bound approximation has been applied to more complex systems (Burkhardt 1976a, Burkhardt and Swendsen 1976, Burkhardt *et al* 1976, Dasgupta 1976, Ashley and Green 1976). In almost all cases, the approximation yielded results which compared very favourably with those obtained by alternative renormalisation group calculations and/or more conventional methods.

These successes suggest that the method of optimised bounds is an extremely powerful and accurate approximation to renormalisation group transformations. However, the *reasons* for this success are far from clear. Indeed, several questions need to be resolved before this approach can be fully assessed and its results accepted without reservation.

Firstly, there is evidence (Plischke and Austin unpublished, Barber 1977c) which suggests that the Kadanoff approximation is not nearly so successful when applied to two-dimensional lattices other than the square. This raises the question of what characteristics are required of an approximation and/or transformation to give good results.

Secondly, as stressed by Kadanoff *et al* (1976), a good bound on the free energy does not imply that the derivatives of the free energy should be approximated at all well by the derivatives of the bound. Yet, it is the behaviour of these derivatives which is characterised by the critical exponents. Thus one would like to know if Kadanoff's results are fortuitous or does the use of renormalisation group techniques somehow ensure, in general, that a good bound to the exact free energy also reproduces the singular behaviour of the derivatives of the free energy? To explore this question, we have elsewhere (Barber 1977a) constructed a simple upper bound approximation for which the optimal transformation could be determined analytically. This optimal transformation, which is equivalent to a site–cell transformation of the form introduced by Niemeijer and van Leeuwen (1973, 1974), again yielded quite accurate exponents for the Ising model on the square lattice but less accurate on other lattices.

More significantly, it was found that the criterion proposed by Kadanoff (1975) to determine the 'best' fixed point out of the set admitted by the approximate recursion relations failed. This criterion, which is discussed in more detail in § 5, had already been called into question by Burkhardt (1976b). In particular, Burkhardt showed that the fixed point located by Kadanoff (1975) possesses a third relevant eigenvalue and is approached only by a special class of Hamiltonians. This class does not include the conventional nearest-neighbour Ising model on the square lattice unless a decimation transformation (Kadanoff and Houghton 1975, Sneddon and Barber 1977) is first performed. The approximate recursion relations of the lower bound transformation do however possess an additional fixed point with a two-dimensional critical surface. Presumably it is to this fixed point that the critical Ising model flows under iteration. Unfortunately, the critical exponents (particularly ν) associated with this point are not as accurate as those of the original point found by Kadanoff.

A resolution of these difficulties and a more complete assessment of the successes of the variational approach, requires a more detailed investigation of the underlying combination of renormalisation group and variational techniques. This is our aim in this series of papers. In this present paper we focus attention on the basic mathematical question: how should the variational parameter(s) be chosen at each iteration of the recursion relation, to ensure that the resulting bound on the free energy (defined as a sum over a renormalisation group trajectory) is optimum? We shall see that this problem is very similar to problems which arise in operations research. Consequently many of the powerful techniques of modern control theory, such as dynamic programming or the Pontryagin maximum principle can be fruitfully applied.

Our detailed arguments are arranged as follows. In § 2 we briefly review the calculation of free energies by renormalisation group techniques and formulate the variational principle. Sections 3 and 4 are devoted to a general treatment of the optimisation problem using techniques from control theory. In § 5 we discuss the

determination of the 'best' fixed point and amplify the remarks made above concerning the Kadanoff criterion. The application of these ideas to the Kadanoff lower bound transformation is discussed in a subsequent paper.

2. Formulation of variational principle

The calculation of free energies by renormalisation group techniques has been discussed by several authors (see e.g. Nauenberg and Nienhuis 1974, Niemeijer and van Leeuwen 1976, van Leeuwen 1975, Kadanoff *et al* 1976). We begin this section by briefly reviewing this theory.

Let $H\{\sigma\}$ denote the Hamiltonian of the system of interest, which we assume to be specified by a set $\{\sigma\}$ of N degrees of freedom or statistical variables. Now consider a transformation of H of the form:

$$\exp(-Ng + H'\{\mu\}) = \mathrm{Tr}_\sigma \mathcal{T}\{\mu, \sigma\} \exp(H\{\sigma\}), \tag{2.1}$$

where the trace is over all states of the system. The new or renormalised Hamiltonian H' describes a system of $N' = N/b^d$ degrees of freedom specified by the set $\{\mu\}$. The parameter b is the spatial re-scaling factor and exceeds unity. Equation (2.1) defines a renormalisation group transformation if $H'\{\mu\}$ possess the same symmetries as $H\{\sigma\}$ and

$$\mathrm{Tr}_\mu \mathcal{T}\{\mu, \sigma\} = 1. \tag{2.2}$$

We shall refer to $\mathcal{T}\{\mu, \sigma\}$ as the *transformation matrix*. The choice of $\mathcal{T}\{\mu, \sigma\}$ is to a large extent arbitrary, although we shall assume that it is non-linear in the new variables $\{\mu\}$, and thus defines a non-linear renormalisation group in the sense of Bell and Wilson (1974). Finally the function $g = g(H)$ is the constant term, i.e. independent of the degrees of freedom, which is generated by the trace over $\{\sigma\}$. (Without loss of generality, we can assume that the total energy is shifted, so that the corresponding term in the original Hamiltonian vanishes.)

Formally, we can write (2.1) as a (non-linear) map on the space of Hamiltonians, namely

$$H' = \mathbb{R}_b H. \tag{2.3}$$

The condition (2.2) then ensures that the free energy per degree of freedom

$$f(H) = \lim_{N\to\infty} \left(-\frac{1}{N} \ln \mathrm{Tr}_\sigma \exp(H\{\sigma\}) \right). \tag{2.4}$$

satisfies

$$f(H) = g(H) + b^{-d} f(\mathbb{R}_b H). \tag{2.5}$$

Iterating this result n times yields

$$f(H) = \sum_{l=0}^{n-1} b^{-ld} g(H_l) + b^{-nd} f(H_n). \tag{2.6}$$

The sequence $\{H_l\}_{l=0}^{n}$ is generated by successive applications of the recursion operator $\mathbb{R}_b$, i.e.

$$H_l = \mathbb{R}_b H_{l-1}, \qquad H_0 \equiv H, \tag{2.7}$$

and terminates when H_n is such that $f(H_n)$ can be readily and accurately evaluated directly from the definition (2.4) by some suitable approximation. In practice, for almost all initial Hamiltonian H, the sequence $\{H_l\}$ tends either to a strong-coupling (low temperature) fixed point or to a weak-coupling (high temperature) fixed point. The exceptions occur when H lies on the critical surface of a non-trivial fixed point H^* of $\mathbb{R}_b$. The corresponding limiting free energy $f(H^*)$ follows immediately from (2.5), namely

$$f(H^*) = (1 - b^{-d})^{-1} g(H^*). \tag{2.8}$$

This approach to the evaluation of free energies has been carried through exactly for the one-dimensional Ising model (Nelson and Fisher 1975, Nauenberg 1975, Priest 1975), the one-dimensional classical Heisenberg model (Niemeijer and Ruijgrok 1975) and approximately for the two-dimensional Ising model (Nauenberg and Nienhuis 1974, Nienhuis and Nauenberg 1975). The basic problem is the evaluation of (2.1) and the determination of an explicit representation (usually as a finite set of non-linear difference equations) of the recursion operator $\mathbb{R}_b$. Knowledge of $\mathbb{R}_b$ is, of course, also necessary for the determination of the type and nature of the critical points of the system of interest; this information following from the fixed points of (2.3). (For recent reviews of renormalisation group theory and techniques see Wilson and Kogut (1974), Fisher (1974), Niemeijer and van Leeuwen (1976), and Barber (1977b).)

Unfortunately, it appears that is only possible to derive an exact representation of $\mathbb{R}_b$ for some one-dimensional examples (see e.g. Nelson and Fisher 1975, Nauenberg 1975, Niemeijer and Ruijgrok 1975). Thus one is forced to evaluate the trace in (2.1) by some approximate procedure†. The various approximations used to date have been reviewed recently by Niemeijer and van Leeuwen (1976). Although these methods have yielded quite accurate results when applied to the two-dimensional Ising model, they do suffer from several serious weaknesses and disadvantages due to their *ad hoc* and unsystematic nature. In particular, physical quantities such as critical exponents depend upon the choice of $\mathcal{T}\{\mu, \sigma\}$. On the other hand, the analysis of Bell and Wilson (1974) for the Gaussian model, suggests that the physical consequences of an *exact* treatment of (2.1) would be independent of $\mathcal{T}$ at least for 'reasonable' choices. It is primarily this problem that a variational approximation attempts to overcome by giving an objective criterion for the 'best' choice of the transformation matrix.

To be more specific, we assume that the allowable choices (for fixed spatial re-scaling factor) of $\mathcal{T}\{\mu, \sigma\}$ can be parametrised by a set of t parameters $\boldsymbol{p}$ and let $\mathbb{R}_b^{\mathrm{A}}(\boldsymbol{p})$ denote the *approximate* recursion operator obtained from (2.1) by some method. (For particular examples see Kadanoff *et al* 1976, Barber 1977a.) This approximation is required to have the property that either

$$f(H) \leqslant g_{\mathrm{A}}(H; \boldsymbol{p}) + b^{-d} f(H'_{\mathrm{A}}(\boldsymbol{p})) \tag{2.9}$$

or

$$f(H) \geqslant g_{\mathrm{A}}(H; \boldsymbol{p}) + b^{-d} f(H'_{\mathrm{A}}(\boldsymbol{p})), \tag{2.10}$$

where

$$H'_{\mathrm{A}}(\boldsymbol{p}) = \mathbb{R}_b^{\mathrm{A}}(\boldsymbol{p}) H \tag{2.11}$$

† We are only interested in non-linear real-space renormalisation groups for which the spatial (d) and spin (n) dimensionalities are fixed. Hence systematic expansions in $\epsilon = 4 - d$ or $1/n$ which yield exact recursion relations are inapplicable.

and $g_A(H; \boldsymbol{p})$ is the appropriate constant term arising in the approximate evaluation of (2.1).

The best choice of $\mathcal{T}\{\mu, \sigma\}$, specified by $\boldsymbol{p} = \boldsymbol{p}^\dagger$, can be determined by adjusting the parameters $\boldsymbol{p}$ variationally to yield the optimum bound in (2.9) or (2.10). Explicitly, in the case of an upper bound approximation, we have

$$f(H) \leqslant f_A(H) = \min_{\boldsymbol{p}} (g_A(H; \boldsymbol{p}) + b^{-d} f(H'_A(\boldsymbol{p})), \tag{2.12}$$

with $\boldsymbol{p}^\dagger$ that value of $\boldsymbol{p}$ for which the minimum is attained.

Since (2.12) involves an optimisation over the unknown exact free energy functional $f(\cdot)$, it is not particularly useful as it stands. To eliminate f it is necessary to iterate, as in the derivation of (2.6), to yield

$$f(H) \leqslant f_A(H) = \min_{\boldsymbol{p}} \Big(\sum_{l=0}^{n-1} b^{-ld} g_A(H_l^A; \boldsymbol{p}) + b^{-nd} f(H_n^A) \Big). \tag{2.13}$$

The sequence $\{H_l^A\}_{l=0}^n$ is now generated by $\mathbb{R}_b^A(\boldsymbol{p})$, i.e.

$$H_l^A = \mathbb{R}_b^A(\boldsymbol{p}) H_{l-1}^A, \qquad H_0^A \equiv H \tag{2.14}$$

and is to terminate when H_n^A is such that $f(H_n^A)$ can be directly evaluated from (2.4).

In writing (2.13) we have tacitly assumed that the optimal transformation of H is independent of H. In general, this need not be the case. (It is not, for example, in the Kadanoff lower bound approximation.) Thus the least upper bound to $f(H)$ is given not by (2.13) but by

$$f(H) \leqslant f_A(H) = \min_{\{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n\}} \Big(\sum_{l=0}^{n-1} b^{-ld} g_A(H_l^A; \boldsymbol{p}_{l+1}) + b^{-nd} f(H_n^A) \Big), \tag{2.15}$$

where $\boldsymbol{p}_k$ denotes the choice of the variational parameters at stage k, i.e.

$$H_k^A = \mathbb{R}_b^A(\boldsymbol{p}_k) H_{k-1}^A, \qquad H_0^A \equiv H. \tag{2.16}$$

Clearly the evaluation of $f_A(H)$ for arbitrary H will be rather non-trivial since it involves a multi-dimensional optimisation. The simplification of this optimisation is a major aim of the following sections. Before turning to this analysis it is useful to ask if the variational parameters $\boldsymbol{p}$ are expected to be subject to any constraints. A detailed answer to this question depends upon the specific approximation. However, all variational approximations developed to date have relied on Jensen's inequality (see e.g. Beckenbach and Bellman 1961). This demands that $\mathcal{T}\{\mu, \sigma\}$ be non-negative and hence $\boldsymbol{p}$ must be chosen to fulfil this condition. Thus, in the following, it should be kept in mind that the components of $\boldsymbol{p}$ may be subject to certain constraints. The existence of constraints has one important consequence. Namely, changes in $\boldsymbol{p}$ from the optimal value $\boldsymbol{p}^\dagger$ need not yield changes in $f_A(H)$ which are second order in $\boldsymbol{p} - \boldsymbol{p}^\dagger$. This point, and some of its implications, will be discussed further in § 5.

3. Bellman equation for $f_A(H)$

According to (2.15), the evaluation of the optimum bound $f_A(H)$ to the exact free energy $f(H)$ for a given Hamiltonian H involves a multi-dimensional optimisation over n vector parameters $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n$. If n is small and the recursion relations relatively easy

to compute, the required optimum can probably be found by a direct numerical search†. However, this method becomes less feasible near criticality, where n will be reasonably large. In addition, such a direct search makes no use of the sequential nature of (2.15) and thus gives little insight into the basic mechanisms of the approximation.

Equation (2.15) has two rather significant and simplifying features. Firstly, the parameters $\boldsymbol{p}_l$ are to be chosen sequentially at each stage of the iteration process. Secondly the function to be optimised consists of a sum of terms, one for each stage of the iteration and each term depending upon a different set of variational parameters. Dynamic programming, developed in the 1950's by Richard Bellman, is explicitly designed to handle such sequential decision processes. In this section we apply the idea of dynamic programming to obtain a simpler equation for $f_{\mathrm{A}}(H)$—the so called Bellman equation. An elementary introduction to dynamic programming has been given by Bellman and Kalaba (1965), while more advanced treatments are contained in Bellman (1957) and Bellman and Dreyfus (1962).

It is convenient, at this stage to modify our notation somewhat. In the usual way, we parametrise the hamiltonians H_l^{A} by appropriate sets of coupling constants, which we shall regard as s-dimensional vectors $\boldsymbol{K}_l = (K_l^1, K_l^2, \ldots, K_l^s)$. The value of s is set by the specific approximation. The recursion relation (2.14) then becomes a set of s first-order difference equations which we write as

$$\boldsymbol{K}' = \boldsymbol{R}(\boldsymbol{K}; \boldsymbol{p}). \tag{3.1}$$

With these changes, the basic result (2.15) becomes

$$f(\boldsymbol{K}) \leqslant f_{\mathrm{A}}(\boldsymbol{K}) = \min_{\{\boldsymbol{p}_1,\ldots,\boldsymbol{p}_n\}} \left(\sum_{l=0}^{n-1} b^{-ld} g(\boldsymbol{K}_l; \boldsymbol{p}_{l+1}) + b^{-nd} f(\boldsymbol{K}_n) \right) \tag{3.2}$$

where

$$\boldsymbol{K}_{l+1} = \boldsymbol{R}(\boldsymbol{K}_l; \boldsymbol{p}_{l+1}), \qquad \boldsymbol{K}_0 \equiv \boldsymbol{K} \tag{3.3}$$

and we have dropped the subscript A on the function g. In the language of control theory, $\boldsymbol{K}$ is the *state-vector*, $\boldsymbol{p}$ is the *control*, while the expression in parenthesis in (3.2) is referred to as the *objective criterion*. We shall, however, continue to use the more conventional terminology of statistical mechanics.

To derive the Bellman equation, we separate out the terms in (3.2) which depend upon $\boldsymbol{p}_1$. Explicitly we can write

$$f_{\mathrm{A}}(\boldsymbol{K}) = \min_{\boldsymbol{p}_1} (g(\boldsymbol{K}, \boldsymbol{p}_1) + \hat{F}), \tag{3.4}$$

where

$$\hat{F} = \min_{\{\boldsymbol{p}_2 \ldots \boldsymbol{p}_n\}} \left(\sum_{l=1}^{n-1} b^{-ld} g(\boldsymbol{K}_l, \boldsymbol{p}_{l+1}) + b^{-nd} f(\boldsymbol{K}_n) \right). \tag{3.5}$$

We observe that F only depends upon $\boldsymbol{p}_1$ through $\boldsymbol{K}_1 = \boldsymbol{R}(\boldsymbol{K}; \boldsymbol{p}_1)$. Thus if $\boldsymbol{K}_1$ is considered to be fixed when the minimization in (3.5) is performed, it immediately follows that

$$\hat{F} = b^{-d} f_{\mathrm{A}}(\boldsymbol{K}_1). \tag{3.6}$$

† This was the procedure adopted by Kadanoff *et al* (1976).

Substituting this result into (3.4) yields

$$f_A(\boldsymbol{K}) = \min_{\boldsymbol{p}}(g(\boldsymbol{K};\boldsymbol{p}) + b^{-d} f_A(\boldsymbol{R}(\boldsymbol{K};\boldsymbol{p})), \tag{3.7}$$

which is the required equation. Note that its derivation depends crucially on the sequential nature of (3.2). The corresponding equation for a lower bound approximation follows similarly, namely

$$f_A(\boldsymbol{K}) = \max_{\boldsymbol{p}}(g(\boldsymbol{K};\boldsymbol{p}) + b^{-d} f_A(\boldsymbol{R}(\boldsymbol{K};\boldsymbol{p}))). \tag{3.8}$$

In both (3.7) and (3.8) the indicated optimisation is, of course, to be performed subject to any constraints.

Although (3.7) is a considerable simplification, in form at least, over (3.2), it has computational limitations due to its functional equation nature. Unless the dimensionality (s) of the space of coupling constants is small, it becomes impossible to solve (3.7) or (3.8) by any iterative procedure because of storage problems. Bellman and Kabala (1965) have termed this problem the 'curse of dimensionality' and it has limited the applicability of dynamic programming. Although, most approximations to renormalisation groups involve too many coupling constants to allow (3.7) or (3.8) to be directly applicable to the variational problem, these equations are, nevertheless, useful. For example, (3.8) can be readily used to show that the Kadanoff lower bound approximation is exact in one dimension (Barber 1977c).

4. Derivation of a Pontryagin maximum principle

To overcome the limitations of dynamic programming, we turn to an alternative approach to control theory, which has developed from the work of Pontryagin in the USSR. The essential feature of this formulation lies in the derivation of a so called Pontryagin maximum principle which determines the optimal control (i.e. the optimal choice of variational parameters). Pontryagin's original treatment (Pontryagin *et al* 1962) is applicable to continuous time processes. The extension to discrete-time processes, which are of relevance here, has been discussed by several authors; notably in an intuitive and heuristic way by Fan and Wang (1964) and more rigorously by Boltyanskii (1974). The derivation we give in this section follows the spirit of a simplified derivation given recently by Blatt (unpublished) for the continuous time case.

Our starting point is again (3.2) and (3.3). Let

$$J = \sum_{l=0}^{n-1} b^{-ld} g(\boldsymbol{K}_l; \boldsymbol{p}_{l+1}) + b^{-nd} f(\boldsymbol{K}_n). \tag{4.1}$$

We wish to *minimise* J over $\{\boldsymbol{p}_1, \ldots \boldsymbol{p}_n\}$ where

$$\boldsymbol{K}_l = \boldsymbol{R}(\boldsymbol{K}_{l-1}; \boldsymbol{p}_l) \tag{4.2}$$

with $\boldsymbol{K}_0$ specified and $\boldsymbol{K}_n$ considered to be free. The parameters $\boldsymbol{p}_l$ at each stage are assumed to be drawn from some set Ω which incorporates any constraints.

To perform this minimisation, we introduce Lagrange multipliers $\boldsymbol{\lambda}_l$, $l = 1, \ldots n$, and consider the Lagrangian

$$\mathcal{L} = J + \sum_{l=1}^{n} \boldsymbol{\lambda}_l \cdot (\boldsymbol{K}_l - \boldsymbol{R}(\boldsymbol{K}_{l-1}; \boldsymbol{p}_l)). \tag{4.3}$$

Defining the Pontryagin function†

$$\Pi_l(\boldsymbol{K}_{l-1}, \boldsymbol{p}_l, \boldsymbol{\lambda}_l) = \boldsymbol{\lambda}_l \cdot \boldsymbol{R}(\boldsymbol{K}_{l-1}; \boldsymbol{p}_l) - b^{-(l-1)d} g(\boldsymbol{K}_{l-1}; \boldsymbol{p}_l), \tag{4.4}$$

$\mathscr{L}$ becomes

$$\mathscr{L} = \sum_{l=1}^{n} (\boldsymbol{\lambda}_l \cdot \boldsymbol{K}_l - \Pi_l(\boldsymbol{K}_{l-1}, \boldsymbol{p}_l, \boldsymbol{\lambda}_l)) + b^{-nd} f(\boldsymbol{K}_n). \tag{4.5}$$

The fundamental theorem of Lagrange multipliers (see e.g. Luenberger 1973) now asserts that minimising J is equivalent to minimising $\mathscr{L}$ with respect to $\boldsymbol{K}_l$ and $\boldsymbol{p}_l$ ($l = 1, \ldots n$) *treated as independent variables.*

Variations with respect to the components of $\boldsymbol{K}_l$ are straightforward. The necessary condition

$$\frac{\partial \mathscr{L}}{\partial K_l^\alpha} = 0 \qquad l = 1, \ldots, n; \alpha = 1, \ldots, s \tag{4.6}$$

yields an equation for $\boldsymbol{\lambda}_l$. Explicitly we find, on differentiating (4.5), that

$$\lambda_l^\alpha = \frac{\partial}{\partial K_l^\alpha} \Pi_{l+1}(\boldsymbol{K}_l, \boldsymbol{p}_{l+1}, \boldsymbol{\lambda}_{l+1}) \qquad l = 1, \ldots, n-1 \tag{4.7}$$

with

$$\lambda_n^\alpha = -b^{-nd} \frac{\partial f(\boldsymbol{K}_n)}{\partial K_n^\alpha}, \qquad \alpha = 1, \ldots, s. \tag{4.8}$$

These equations will be referred to as the co-state equations. Note also that the recursion relations (4.2) follow from Π_l as

$$K_l^\alpha = \frac{\partial}{\partial \lambda_l^\alpha} \Pi_l(\boldsymbol{K}_{l-1}, \boldsymbol{p}_l, \boldsymbol{\lambda}_l). \tag{4.9}$$

Turning now to variations in $\boldsymbol{p}_l$, we find on the assumption that $\mathscr{L}$ is differentiable with respect to $\boldsymbol{p}$, that a necessary condition for optimality is

$$\frac{\partial \mathscr{L}}{\partial p_l^\alpha} = -\frac{\partial}{\partial p_l^\alpha} \Pi_l = 0. \tag{4.10}$$

Thus $\boldsymbol{p}_l^\dagger$ is determined by the condition that the Pontryagin function $\Pi_l(\boldsymbol{p}_l)$ at stage l be extremal at $\boldsymbol{p}_l = \boldsymbol{p}_l^\dagger$. However if the parameters $\boldsymbol{p}_l$ are constrained, the solution of (4.10) may violate the constraints and hence be inadmissible. To cover this possibility, one must argue rather differently. In doing so, we can, in fact, establish the stronger result that at optimality, Π_l is a *maximum* with respect to $\boldsymbol{p}_l$.

Let $\boldsymbol{p}_1^\dagger, \boldsymbol{p}_2^\dagger, \ldots, \boldsymbol{p}_n^\dagger$ denote the optimal choice of variational parameters and $\boldsymbol{K}_0, \boldsymbol{K}_1^\dagger, \boldsymbol{K}_2^\dagger, \ldots, \boldsymbol{K}_n^\dagger$, the corresponding sequence of coupling constants. Now consider the sub-optimal choice

$$\boldsymbol{p}_1^\dagger, \boldsymbol{p}_2^\dagger, \ldots, \boldsymbol{p}_{k-1}^\dagger, \boldsymbol{p}_k = \boldsymbol{p}_k^\dagger + \boldsymbol{\xi}, \boldsymbol{p}_{k+1}^\dagger, \ldots, \boldsymbol{p}_n^\dagger. \tag{4.11}$$

where we assume that $\boldsymbol{p}_k$ can be chosen (subject to any constraints) to make $\boldsymbol{\xi}$ arbitrarily small. This assumption is valid if the set, Ω, of allowed values of the variational parameters $\boldsymbol{p}$, is continuous and directionally convex as is the case in renormalisation group calculations.

† In control theory Π_l is usually denoted H_l and called the (Pontryagin) Hamiltonian. We have chosen the alternative notation to avoid confusion with the conventional Hamiltonian of statistical mechanics.

The new sequence of coupling constants is

$$\boldsymbol{K}_l = \begin{cases} \boldsymbol{K}_l^\dagger & 0 \leqslant l \leqslant k-1 \\ \boldsymbol{R}(\boldsymbol{K}_{k-1}^\dagger; \boldsymbol{p}_k^\dagger + \boldsymbol{\xi}) & l = k \\ \boldsymbol{R}(\boldsymbol{K}_{l-1}; \boldsymbol{p}_l^\dagger) & k+1 \leqslant l \leqslant n. \end{cases} \tag{4.12}$$

Provided $\boldsymbol{R}$ is differentiable with respect to $\boldsymbol{p}$ we have

$$\boldsymbol{K}_k = \boldsymbol{K}_k^\dagger + \mathrm{O}(\boldsymbol{\xi}) \tag{4.13}$$

and hence by induction

$$\delta\boldsymbol{K}_l \equiv \boldsymbol{K}_l - \boldsymbol{K}_l^\dagger = \mathrm{O}(\boldsymbol{\xi}) \tag{4.14}$$

for all $l \geqslant k$. Turning to the co-state equation (4.7), we observe from (4.8) and (4.14) that

$$\delta\boldsymbol{\lambda}_n = \boldsymbol{\lambda}_n - \boldsymbol{\lambda}_n^\dagger = \mathrm{O}(\boldsymbol{\xi}) \tag{4.15}$$

and hence on iterating (4.7) backwards we conclude that

$$\delta\boldsymbol{\lambda}_l = \boldsymbol{\lambda}_l - \boldsymbol{\lambda}_l^\dagger = \mathrm{O}(\boldsymbol{\xi}), \qquad 1 \leqslant l \leqslant n. \tag{4.16}$$

We are now in a position to compute the difference between the values of the Lagrangian (4.5) calculated using the optimal choice of the $\boldsymbol{p}$'s and that obtained from (4.11). We write

$$\begin{aligned} \mathscr{L} - \mathscr{L}^\dagger = \sum_{\substack{l=1 \\ l \neq k}}^{n} & (\boldsymbol{\lambda}_l \,.\, \boldsymbol{K}_l - \boldsymbol{\lambda}_l^\dagger \,.\, \boldsymbol{K}_l^\dagger - \Pi_l(\boldsymbol{K}_{l-1}, \boldsymbol{p}_l^\dagger, \boldsymbol{\lambda}_l) + \Pi_l(\boldsymbol{K}_{l-1}^\dagger, \boldsymbol{p}_l^\dagger, \boldsymbol{\lambda}_l^\dagger)) \\ & + \boldsymbol{\lambda}_k \,.\, \boldsymbol{K}_k - \boldsymbol{\lambda}_k^\dagger \,.\, \boldsymbol{K}_k^\dagger - \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k) + \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k^\dagger, \boldsymbol{\lambda}_k^\dagger) \\ & + b^{-nd}(f(\boldsymbol{K}_n) - f(\boldsymbol{K}_n^\dagger)). \end{aligned} \tag{4.17}$$

From (4.7), (4.9) and the estimates (4.14), (4.16), we have

$$\Pi_l(\boldsymbol{K}_{l-1}, \boldsymbol{p}_l^\dagger, \lambda_l) - \Pi_l(\boldsymbol{K}_{l-1}^\dagger, \boldsymbol{p}_l^\dagger, \boldsymbol{\lambda}_l^\dagger) = \boldsymbol{\lambda}_{l-1}^\dagger \,.\, \delta\boldsymbol{K}_{l-1} + \boldsymbol{K}_l^\dagger \,.\, \delta\boldsymbol{\lambda}_l + \mathrm{O}(\xi^2), \tag{4.18}$$

where by $\mathrm{O}(\xi^2)$ we include any term quadratic in the components of $\boldsymbol{\xi}$. Similarly

$$b^{-nd}(f(\boldsymbol{K}_n) - f(\boldsymbol{K}_n^\dagger)) = -\boldsymbol{\lambda}_n^\dagger \,.\, \delta\boldsymbol{K}_n + \mathrm{O}(\xi^2) \tag{4.19}$$

and

$$\boldsymbol{\lambda}_l \,.\, \boldsymbol{K} - \boldsymbol{\lambda}_l^\dagger \,.\, \boldsymbol{K}_l^\dagger = \boldsymbol{\lambda}_l^\dagger \,.\, \delta\boldsymbol{K}_l + \boldsymbol{K}_l^\dagger \,.\, \delta\boldsymbol{\lambda}_l + \mathrm{O}(\xi^2). \tag{4.20}$$

Substituting these results in (4.17) yields

$$\mathscr{L} - \mathscr{L}^\dagger = \boldsymbol{K}_k^\dagger \,.\, \delta\boldsymbol{\lambda}_k + \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k^\dagger, \boldsymbol{\lambda}_k^\dagger) - \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k) + \mathrm{O}(\xi^2) \tag{4.21}$$

where we have used the fact that $\boldsymbol{K}_l \equiv \boldsymbol{K}_l^\dagger$ for $l \leqslant k-1$. (Note however that $\boldsymbol{\lambda}_l \neq \boldsymbol{\lambda}_l^\dagger$ for $l \leqslant k-1$.) Equation (4.21) can be rewritten as

$$\begin{aligned} \mathscr{L} - \mathscr{L}^\dagger = \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k^\dagger, \boldsymbol{\lambda}_k^\dagger) - \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k^\dagger) + \boldsymbol{K}_k^\dagger \,.\, \delta\boldsymbol{\lambda}_k + \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k - \delta\boldsymbol{\lambda}_k) \\ - \Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k) + \mathrm{O}(\xi^2). \end{aligned} \tag{4.22}$$

But

$$\Pi_k(\boldsymbol{K}_{k-1}^\dagger, \boldsymbol{p}_k, \boldsymbol{\lambda}_k - \delta\boldsymbol{\lambda}_k) - \Pi_k(\boldsymbol{K}_{k-1}, \boldsymbol{p}_k, \lambda_k) = -\boldsymbol{K}_k \,.\, \delta\boldsymbol{\lambda}_k + \mathrm{O}(\xi^2) = -\boldsymbol{K}_k^\dagger \,.\, \delta\boldsymbol{\lambda}_k + \mathrm{O}(\xi^2) \tag{4.23}$$

and hence we finally obtain

$$\mathscr{L}-\mathscr{L}^{\dagger}=\Pi_k(\boldsymbol{K}_{k-1}^{\dagger},\boldsymbol{p}_k^{\dagger},\boldsymbol{\lambda}_k^{\dagger})-\Pi_k(\boldsymbol{K}_{k-1}^{\dagger},\boldsymbol{p}_k,\boldsymbol{\lambda}_k^{\dagger})+O(\xi^2). \tag{4.24}$$

However, by assumption $\mathscr{L}^{\dagger}$ is less than $\mathscr{L}$. Thus for sufficiently small variations (in Ω) of $\boldsymbol{p}_k$ from optimality, we conclude that

$$\Pi_k(\boldsymbol{K}_{k-1}^{\dagger},\boldsymbol{p}_k^{\dagger},\boldsymbol{\lambda}_k^{\dagger})\geqslant\Pi_k(\boldsymbol{K}_{k-1}^{\dagger},\boldsymbol{p}_k,\boldsymbol{\lambda}_k^{\dagger}). \tag{4.25}$$

This result is the Pontryagin maximum principle.

The extension to the case of a lower bound approximation is most easily obtained by negating the function g (i.e. we minimise $-f$). The co-state equations (4.7) and the maximum principle (4.19) remain valid with the Pontryagin function now defined as

$$\Pi_l=\boldsymbol{\lambda}_l\,.\,\boldsymbol{R}(\boldsymbol{K}_{l-1};\boldsymbol{p}_l)+b^{-(l-1)d}g(\boldsymbol{K}_{l-1};\boldsymbol{p}_l). \tag{4.26}$$

Several comments are now appropriate. Firstly, it should be noted that the maximum principle is only a *necessary* condition for optimality. In addition, we have not established the existence or uniqueness of the optimal choice of the variational parameters. These questions are however not of great concern in the application of these ideas to renormalisation group approximations. Of more importance is the possibility of actually *solving* the Pontryagin equations, which consist of (4.2), (4.7) and (4.25).

The derivation of the maximum principle, given above, tacitly assumes that the number of iterations n is fixed and $\boldsymbol{K}_n$ is free. Actually, n is determined by the condition that $\boldsymbol{K}_n$ is non-critical in the sense that $f(\boldsymbol{K}_n)$ can be evaluated directly from the definition (2.4) (see the discussion after (2.7)). Consequently, $\boldsymbol{\lambda}_n$ defined by (4.8) can be considered to be known and thus $\boldsymbol{\lambda}_l$ determined by iterating (4.7) backwards. However, this procedure is somewhat cumbersome to implement. Instead it seems sufficient to choose a fixed value of n sufficiently large to allow λ_n^{α} to be taken as zero. An estimate of this value of n can be obtained as follows. Differentiating (2.4) yields

$$\frac{\partial f}{\partial K^{\alpha}}=\lim_{N\to\infty}\left(-\frac{1}{N}\langle\partial H/\partial K^{\alpha}\rangle\right), \tag{4.27}$$

where the angular brackets denote an ensemble average. We now assume that K^{α} denotes the coupling between a sub-set of the degrees of freedom, denoted α, and appears in H in the form:

$$K_{\alpha}\sum S_{\alpha},\qquad S_{\alpha}=\prod_{i\in\alpha}\sigma_i^{m_{i,\alpha}}, \tag{4.28}$$

where the sum runs over all embeddings of α in the complete set $\{\sigma_i\}$ and $m_{i,\alpha}$ is a positive integer. Hence

$$\lambda_n^{\alpha}=c_{\alpha}b^{-nd}\langle S_{\alpha}\rangle, \tag{4.29}$$

where c_{α} is a numerical constant which counts the number of embeddings of α per degree of freedom. To proceed requires a more detailed specification of the system. For an Ising model ($\sigma_i=\pm1$, $i=1,\ldots,N$), we immediately have

$$|\lambda_n^{\alpha}|\leqslant c_{\alpha}b^{-nd}. \tag{4.30}$$

A similar bound follows if we assume the σ_i and hence S_{α} are bounded. Although we have not explored the possibility of applying these results to continuous spin systems ($-\infty<\sigma_i<\infty$), we note that Ruelle (1976) has recently proved that $\langle S_{\alpha}\rangle$ is bounded for

such systems. In general, it therefore appears that λ_n^α tends to zero exponentially as n tends to infinity. In practice, it is thus sufficient to fix n at say 15–25 and assume λ_n^α to be identically zero. This approach has been used to successively solve the Pontryagin equations for the Kadanoff lower bound approximation (Barber and Kelley 1977).

5. Fixed point criteria

The preceding two sections have concerned the optimisation problem posed by (2.15). However, the actual evaluation of $f_A(H)$ for arbitrary H is often of little interest. Rather we require the fixed points and related scaling fields and exponents of the optimal transformation. The question arises as to whether or not this information can be obtained without recourse to the full computation of $f_A(H)$.

Kadanoff (1975) suggested that this was possible and proposed a simple criterion to determine the 'best' fixed point. To derive the Kadanoff criterion it is necessary to make two assumptions:

(i) Given $\boldsymbol{K}_0 = \boldsymbol{K}$, we assume that the subsequent optimal sequence of coupling constants $\{\boldsymbol{K}_l^\dagger\}$ is generated by a *constant fixed value of the variational parameter vector*, say $\boldsymbol{p}^\dagger = \boldsymbol{p}^\dagger(\boldsymbol{K})$.

(ii) Either $\boldsymbol{p}$ is assumed to be unconstrained or if it is constrained to some set Ω, we assume that the optimal choice $\boldsymbol{p}^\dagger$ corresponds to an internal optimum.

Explicitly this second assumption means that if $\boldsymbol{p}$ is subject to any inequality constraints then $\boldsymbol{p}^\dagger$ must satisfy these constraints with *strict* inequality.

Let

$$\psi(\boldsymbol{K}, \boldsymbol{p}) = \sum_{l=0}^{\infty} b^{-ld} g(\boldsymbol{K}_l; \boldsymbol{p}) \tag{5.1}$$

with

$$\boldsymbol{K}_l = \boldsymbol{R}(\boldsymbol{K}_{l-1}; \boldsymbol{p}) \tag{5.2}$$

and define

$$\psi_A(\boldsymbol{K}) = \operatorname*{opt}_{\boldsymbol{p}}(\psi(\boldsymbol{K}, \boldsymbol{p})), \tag{5.3}$$

where 'opt' denotes a maximisation or minimisation as is appropriate. Note that $\psi_A(\boldsymbol{K})$ will not, in general, equal the bound $f_A(\boldsymbol{K})$ given by (2.15), since $\boldsymbol{p}_l^\dagger$ is, in general, *not* constant for all l. For an upper bound approximation we have

$$\psi_A(\boldsymbol{K}) \geqslant f_A(\boldsymbol{K}) \geqslant f(\boldsymbol{K}), \tag{5.4}$$

where $f(\boldsymbol{K})$ is the exact free energy, while the inequalities in (5.4) are reversed for a lower bound approximation.

The second of Kadanoff's assumptions now allows us to assert that $\psi_A(\boldsymbol{K})$ corresponds to a stationary point of $\psi(\boldsymbol{K}, \boldsymbol{p})$ with respect to variations in $\boldsymbol{p}$ from $\boldsymbol{p}^\dagger$. Explicitly we have

$$\Delta\psi = \psi(\boldsymbol{K}, \boldsymbol{p}^\dagger + \delta\boldsymbol{p}) - \psi(\boldsymbol{K}, \boldsymbol{p}^\dagger) = O((\delta\boldsymbol{p})^2). \tag{5.5}$$

This result is valid for all $\boldsymbol{K}$; in particular it is required to be true for the fixed point $\boldsymbol{K}^* = \boldsymbol{K}^*(\boldsymbol{p}^\dagger)$, which satisfies

$$\boldsymbol{K}^* = \boldsymbol{R}(\boldsymbol{K}^*; \boldsymbol{p}^\dagger). \tag{5.6}$$

Thus (5.5) gives a criterion for selecting a 'best' fixed point from the set $\{\boldsymbol{K}^*(\boldsymbol{p})\}$ of fixed points admitted by the approximate recursion relations for arbitrary value of $\boldsymbol{p}$.

If

$$\boldsymbol{p}^\dagger = (p_1^\dagger, p_2^\dagger, \ldots, p_t^\dagger), \tag{5.7}$$

then we show in the appendix that $p_m^\dagger$ satisfies

$$(\partial g/\partial p_m)^* + (\partial g/\partial \boldsymbol{K})^* \cdot (b^d \boldsymbol{I} - \boldsymbol{T})^{-1} \cdot (\partial \boldsymbol{R}/\partial p_m)^* = 0, \qquad m = 1, \ldots, t, \tag{5.8}$$

where $\boldsymbol{I}$ is the s-dimensional unit matrix and the matrix $\boldsymbol{T}$ has components

$$T_{\alpha\beta} = (\partial R^\alpha/\partial K^\beta)^* \qquad \alpha = 1, \ldots, s; \beta = 1, \ldots, s. \tag{5.9}$$

The asterisk in (5.8) and (5.9) indicates that the derivatives are to be evaluated at $\boldsymbol{K} = \boldsymbol{K}^*(\boldsymbol{p}^\dagger)$ and $\boldsymbol{p} = \boldsymbol{p}^\dagger$. Equation (5.8) is the Kadanoff criterion (Kadanoff 1975, Kadanoff *et al* 1976).

The criterion has formed the basis of all the highly successful applications of the Kadanoff lower bound approximations cited in § 1. For example, for the two-dimensional Ising model on the square lattice, it leads to the estimates (Kadanoff 1975)

$$\delta = 15{\cdot}04, \qquad \nu = 0{\cdot}9991, \tag{5.10}$$

which compare very favourably with the exact value of 15 and 1 respectively. As mentioned in § 1 there are, however, several problems associated with this procedure.

Firstly, Barber (1977a) has constructed a class of upper bound approximations for which the criterion fails. This failure is a consequence of the optimal transformation satisfying an inequality constraint with equality. Thus assumption (ii) is invalid.

Secondly, the criterion gives no grounds to select between multiple solutions of (5.8). Since (5.6) is a set of non-linear equations, it can very easily possess more than one fixed point $\boldsymbol{K}^*$ for a particular value of $\boldsymbol{p}$. Burkhardt (1976b) and Knops (1977) have shown that this problem actually arises in the Kadanoff lower bound approximation; the criterion (5.8) giving *three* possible 'optimal' fixed points with different values of the critical exponents.

Thirdly, there is the inconsistency noted by Kadanoff *et al* (1976), which arises when the recursion operator is linearised about the fixed point with $\boldsymbol{p}$ fixed at the fixed point value $\boldsymbol{p}^\dagger$. Knops (1977) has recently discussed this problem on the basis of a simple linear treatment of the correction terms and found that the values of the critical exponents change rather significantly. The effect appears to be so large as to call into question the assumption, made by Knops, that a linear analysis is sufficient.

Finally, there is the fundamental problem associated with the first assumption of the Kadanoff criterion. Since Kadanoff *et al* (1976) have show that significantly better results are obtained for thermodynamic functions if the variational parameters are allowed to vary along a flow trajectory, it appears that this assumption is very stringent.

The only way that these problems can be resolved is by a more detailed computation of optimal parameters for at least a subset of initial Hamiltonians. Hence we are led back to the optimisation problem posed by (2.15). This problem has, however, been considerably simplified by the analysis of the two preceding sections. In particular, the Pontryagin maximum principle of § 4 can be used to rapidly, accurately and *unambiguously* determine the critical temperature and related fixed point of physical Hamiltonians. Details of this calculation for the Kadanoff approximation will be published elsewhere (Barber and Kelley 1977). Here we describe the salient features and how they resolve, in general, the difficulties of the Kadanoff criterion.

We consider first the determination of the best fixed point. Let Z^* denote the set

$$Z^* = \{(\boldsymbol{K}, \boldsymbol{p}) | \boldsymbol{K} = \boldsymbol{R}(\boldsymbol{K}; \boldsymbol{p})\}. \tag{5.11}$$

Then for each $(\boldsymbol{K}, \boldsymbol{p}) \in Z^*$, the function $\psi(\boldsymbol{K}, \boldsymbol{p})$ defined by (5.1) is trivial to evaluate:

$$\psi(\boldsymbol{K}, \boldsymbol{p}) = (1 - b^{-d})^{-1} g(\boldsymbol{K}, \boldsymbol{p}), \qquad (\boldsymbol{K}, \boldsymbol{p}) \in Z^*.$$

By assumption the 'best' fixed point $(\boldsymbol{K}^*, \boldsymbol{p}^\dagger)$ must remain invariant under iteration. Thus the optimal choice of variational parameters, given $\boldsymbol{K}_0 = \boldsymbol{K}^*$, *but only this point*, is invariant. Hence we require

$$\psi(\boldsymbol{K}^*, \boldsymbol{p}^\dagger) = f_A(\boldsymbol{K}^*) \tag{5.12}$$

where $f_A(\boldsymbol{K}^*)$ is the optimal bound given by (2.15) (or its obvious analogue for a lower bound approximation) with $\boldsymbol{K}_0 = \boldsymbol{K}^*$. Note that this new criterion does not make any assumption concerning the behaviour of $\psi(\boldsymbol{K}, \boldsymbol{p})$ near $\boldsymbol{p}^\dagger$. Hence unlike the Kadanoff criterion, it is applicable if $\boldsymbol{p}^\dagger$ is a boundary optima. In the case of the upper bound approximations of Barber (1977a), one can show that (5.12) yields the exact optimal transformations.

Equation (5.12) may still and, in general, probably will, admit multiple pairs $(\boldsymbol{K}, \boldsymbol{p})$ from Z^*. To select the physically relevant point requires some knowledge of the critical surface or the domains of attraction of the solutions of (5.12). In practice, it is easier to select a series of initial Hamiltonians $\boldsymbol{K}_0$ in the physical sub-space of the full Hamiltonian space and compute the optimal flow trajectories. This calculation yields both the critical parameters (e.g. critical temperature) of the physical Hamiltonians of interest and the related fixed point without *ambiguity*.

It is worth emphasising that any fixed point of a recursion operator is only of physical relevance if the point in question is accessible from the physical sub-space. This aspect is often overlooked in renormalisation group calculations but appears to be of considerable importance in interpreting variational approximations.

Once the appropriate fixed point pair $(\boldsymbol{K}^*, \boldsymbol{p}^\dagger)$ in Z^* has been located, the required linear transformation can be obtained quite consistently as follows. Choose an initial set of coupling constants

$$\boldsymbol{K}_0 = (K_1^*, K_2^*, \ldots, K_{m-1}^*, K_m^* + \Delta K, K_{m-1}^*, \ldots, K_s^*). \tag{5.13}$$

Calculate $f_A(\boldsymbol{K}_0)$ and let $\boldsymbol{K}_1$ be the first (after $\boldsymbol{K}_0$) of the optimal sequence of coupling parameters. Then the required representation of the linear recursion operator near K^* is approximated by

$$T_{jm} = (K_{1,j} - K_j^*)/\Delta K. \tag{5.14}$$

In practice, it is better to consider both negative and positive variations of K_m^* in (5.13) as this minimises the effects of uncertainty in the determination of K^*. Preliminary calculations along these lines, indicate that errors associated with neglecting the variation in $\boldsymbol{p}\dagger$ and fixing it at its fixed point value are somewhat smaller than found by Knops (1977).

Of course, the whole of the procedure outlined above is only feasible if the optimisation problem posed by (2.15) can be solved rapidly and accurately *even near the fixed point* for which the number of iterations n is relatively large. The analysis of this paper, particularly § 4, makes this possible. Indeed, the amount of computer time

required is not much more than required to compute the Kadanoff criterion (5.8). In a subsequent paper, we shall use these results to attempt a comprehensive assessment of the Kadanoff lower bound approximation.

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Appendix. Derivation of Kadanoff criterion

In this appendix, we show that the Kadanoff criterion (5.8) follows from (5.5). We observe that

$$\psi(\boldsymbol{K}^*, \boldsymbol{p}^\dagger) = (1-b^{-d})^{-1} g(\boldsymbol{K}^*; \boldsymbol{p}^\dagger), \tag{A.1}$$

where $\boldsymbol{K}^*$ satisfies (5.6) with $\boldsymbol{p} = \boldsymbol{p}^\dagger$. Now let $\boldsymbol{K}_0 = \boldsymbol{K}^*$ and consider a change Δp in the mth component of $\boldsymbol{p}^\dagger$. Then from (5.2)

$$\boldsymbol{K}_1 = \boldsymbol{K}^* + \boldsymbol{u}_m \, \Delta p + \mathrm{O}(\Delta p^2) \tag{A.2}$$

with

$$\boldsymbol{u}_m = (\partial \boldsymbol{R}/\partial p_m)^* \tag{A.3}$$

and the asterisk indicating that the derivative is to be evaluated at $\boldsymbol{K} = \boldsymbol{K}^*$ and $\boldsymbol{p} = \boldsymbol{p}^\dagger$.

By induction it then follows that

$$\boldsymbol{K}_l = \boldsymbol{K}^* + \boldsymbol{y}_l \, \Delta p + \mathrm{O}(\Delta p^2) \qquad l = 1, 2, \ldots \tag{A.4}$$

where

$$\boldsymbol{y}_{l+1} = \boldsymbol{u}_m + \boldsymbol{T}\boldsymbol{y}_l, \qquad \boldsymbol{y}_0 = 0 \tag{A.5}$$

and the matrix $\boldsymbol{T} = \boldsymbol{T}(p^\dagger)$ is defined by (5.9). The linear recursion relation (A.5) has solution

$$\boldsymbol{y}_l = (\boldsymbol{I} + \boldsymbol{T}^l)\boldsymbol{y} \tag{A.6}$$

where $\boldsymbol{I}$ is the $s \times s$ unit matrix and $\boldsymbol{y}$ satisfies

$$(\boldsymbol{I} - \boldsymbol{T})\boldsymbol{y} = \boldsymbol{u}_m. \tag{A.7}$$

We are now in a position to compute $\Delta\psi$ to order $(\Delta p)^2$ explicitly. Substituting (A.4) gives

$$g(\boldsymbol{K}_l; p_1^\dagger, p_2^\dagger, \ldots, p_{m-1}^\dagger, p_m + \Delta p, p_{m+1}^\dagger, \ldots, p_l^\dagger)$$
$$= g(\boldsymbol{K}^*; \boldsymbol{p}^\dagger) + (h_m + \boldsymbol{d} \cdot \boldsymbol{y}_l)\Delta p + \mathrm{O}(\Delta p^2) \tag{A.8}$$

where

$$h_m = (\partial g/\partial p_m)^* \tag{A.9}$$

and

$$\boldsymbol{d} = (\partial g/\partial \boldsymbol{K})^* \tag{A.10}$$

is the gradient of g with respect to $\boldsymbol{K}$. Hence

$$\Delta\psi = \Delta p \sum_{l=0}^{\infty} b^{-ld}(h_m + \boldsymbol{y}_l \cdot \boldsymbol{d}) + O(\Delta p^2). \tag{A.11}$$

Equation (5.2) now asserts that $p_m^{\dagger}$ is such that

$$\Omega(p_m) = \sum_{l=0}^{\infty} b^{-ld}(h_m + \boldsymbol{y}_l \cdot \boldsymbol{d}) \equiv 0. \tag{A.12}$$

Substituting (A.6) allows the sum to be evaluated. After some algebra we obtain

$$\Omega(p_m) = (1 - b^{-d})^{-1}[h_m + \boldsymbol{d} \cdot (b^d \boldsymbol{I} - \boldsymbol{T})\boldsymbol{u}_m], \tag{A.13}$$

from which (5.8) follows immediately.

This result is not of the form quoted in Kadanoff *et al* (1976). It is straightforward however, to show that (5.8) and equation (43) of Kadanoff *et al* are identical. To do so, we first note that Kadanoff *et al* incorporate the constant term g into the space of coupling constants, defining $K_0 = -g$. Their linearised transform, specified by a $(s+1)\times(s+1)$ dimensional matrix $\boldsymbol{B}$, is related to $\boldsymbol{T}$ by

$$\boldsymbol{B} = \begin{pmatrix} b^d & -\boldsymbol{d} \\ \boldsymbol{0} & \boldsymbol{T} \end{pmatrix} \tag{A.14}$$

This matrix has an eigenvalue $\Lambda_0 = b^d$ with a trivial left eigenvector. The corresponding right eigenvector we write as $(1, \boldsymbol{v})$ and find that

$$\boldsymbol{v} = -\boldsymbol{d}(b^d \boldsymbol{I} - T)^{-1}. \tag{A.15}$$

Substituting this result in (A.13) immediately reduces it to equation (43) of Kadanoff *et al* (1976).

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