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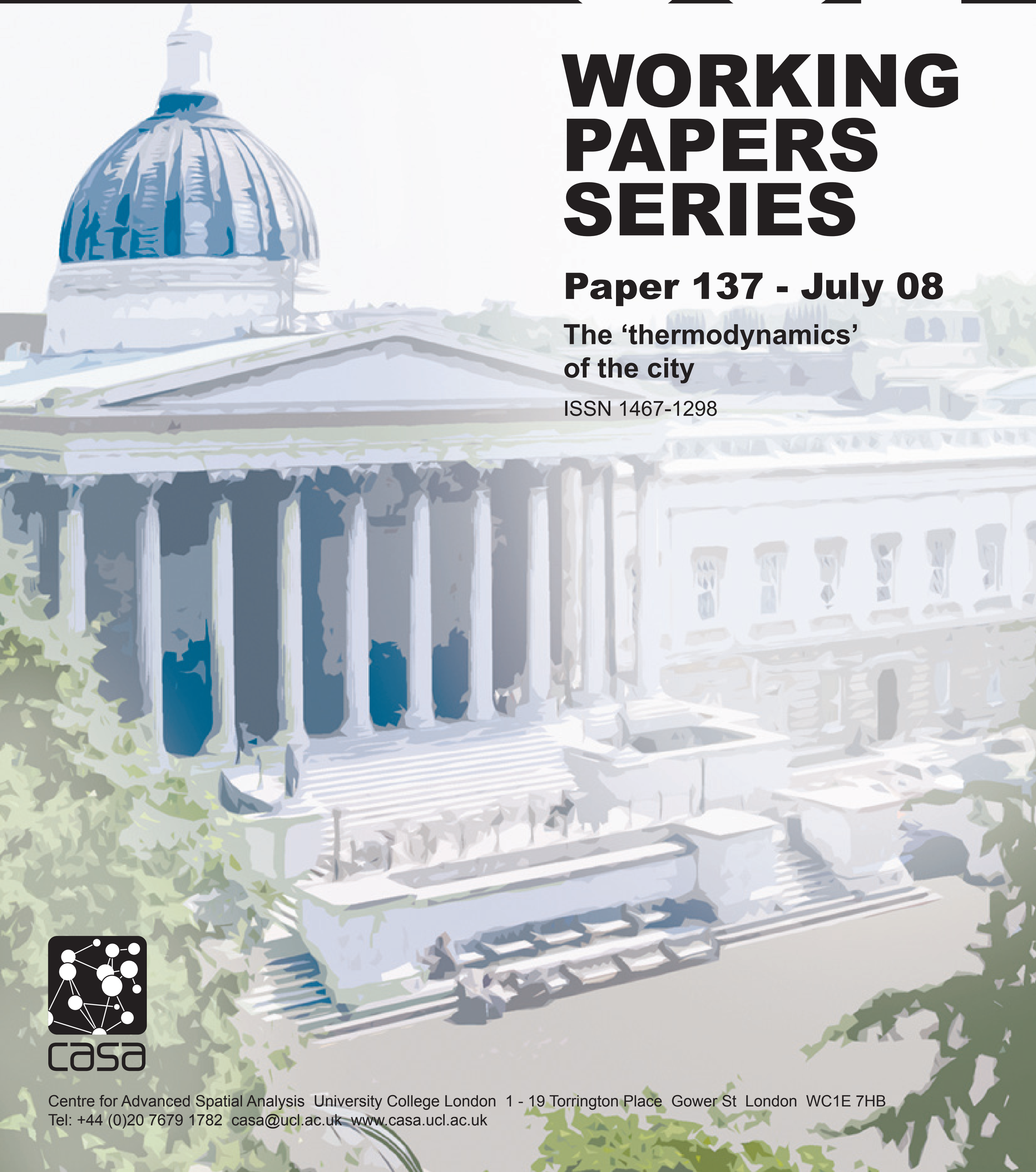

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The 'thermodynamics' of the city

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Centre for Advanced Spatial Analysis University College London 1 - 19 Torrington Place Gower St London WC1E 7HB
Tel: +44 (0)20 7679 1782 casa@ucl.ac.uk www.casa.ucl.ac.uk

The 'thermodynamics' of the city

Alan Wilson

Centre for Advanced Spatial Analysis,
University College London,
London WC1E 7HB

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Abstract

The methods of statistical mechanics have been successfully applied in urban modelling and there has been some attempt at the interpretation of the results in terms of 'thermodynamics'. The aim of this paper is to seek to review these interpretations more systematically, to seek new insights and to chart a programme of future research which would be facilitated by the bringing together of interdisciplinary teams.

1. Introduction.

The primary objectives of this paper are twofold: first, to offer a review of progress in urban modelling using the methods of statistical mechanics; and secondly, to explore the possibility of using the *thermodynamic* analogy in addition to statistical mechanics[1]. We can take stock of the 'thermodynamics of the city' not in the sense of its physical states – interesting though that would be – but in terms of its daily functioning and its evolution over time.

It is becoming increasingly recognised that the mathematics underpinning thermodynamics and statistical mechanics have wide applicability. This is manifesting itself in two ways: broadening the range of systems for which these tools are relevant; and seeing that there are new mathematical insights that derive from this branch of Physics. The recognition of the power of the method and its wider

[1] Taking advantage of the approaches of authors like Ruelle (1991) who see what they call the 'thermodynamic formalism' as a general tool.

application goes back at least to the 1950s (Jaynes, 1957, for example). The methods have been deployed in various mathematical fields: Markov processes, nonlinear dynamics and ergodic theory for instance. The applications have mainly been in fields closely related to the physical sciences. The purpose of this paper is to demonstrate the relevance of the methods in a field that has had less publicity but which is obviously important: the development of mathematical models of cities.

In this context, there have been two main phases of development in urban science and a third now beckons. The first was in the direct application of the methods of statistical mechanics in urban analysis in the modelling of transport patterns in cities (Wilson, 1967). These models were developed by analogy though it was soon recognised that what was being used was a powerful general method. A family of spatial interaction models was derived and one of these was important as the beginnings of locational analysis as well as the representation of flows in transport models (Wilson, 1970).

The second phase extended the locational analysis to the modelling of the evolution of structures, with retail outlets providing an archetypal model (Harris and Wilson, 1978). This was rooted in the developments in applied nonlinear dynamics in the 1970s and not directly connected to statistical mechanics. The equations were largely solved by computer simulation, though some analytical insights were achieved. This provides the beginnings of a method for modelling the evolution of cities – the urban analogue of the equivalent issue in developmental biology.

The emerging third phase reconnects with statistical mechanics. There was always the possibility that analogies with Ising models and their progeny would offer further insights since these represented a kind of locational structure problem in physics and some interesting mathematics were associated with these models. Statistical mechanics is now handling much more complex structural models than the one-dimensional Ising model and there is a much fuller understanding of phase transitions. This makes it worthwhile to pursue the analogy again – especially in exploring the possible existence of phase transitions in urban development.

The paper is structured as follows. In section 2, we briefly outline the systems of interest – broadly, cities and (urban) regions. In section 3, we summarise the key concepts of thermodynamics and statistical mechanics that are relevant for urban and regional modelling. In section 4, we explore the three phases of development of urban modelling, seeking to articulate the 'thermodynamics of the city' wherever it is possible and fruitful. In section 5, we explore future challenges.

2. Cities as systems of interest.

2.1. The archetypal submodels.

Transport planners have long needed to understand the pattern of flows in cities and a core scientific task is to model these flows both to account for an existing situation and to be able to predict the consequences of change in the future – whether through, for example, population change or through planned transport investment and network development. The models in principle provide the analytical base for optimising transport policy and investment.

Assume that the city can be divided into a set of discrete zones, labelled 1, 2, 3, …..N. Then the core of the modelling task is to estimate the array $\{T_{ij}\}$, where T_{ij} is the number of trips from zone i to zone j. This pattern obviously depends on a whole host of variables: trip demand at i (origins, O_i), trip attractions at j (destinations, D_j), the underlying transport network and associated congestion effects, and so on. The network is handled through a matrix of generalised travel costs, $\{c_{ij}\}$. We describe the core model in section 4.2.

Suppose we now focus on retail trips alone, represented by a matrix $\{S_{ij}\}$. These might be proportional to the spending power at i (e_iP_i, with e_i as per capita expenditure, P_i, the population) and the attractiveness of retail facilities in j (which we designate as W_j). The model can then predict a valuable locational vector $\{D_j\}$ which is $\Sigma_i S_{ij}$, the sum of the flows into a retail centre attracted by W_j. An ability to predict $\{D_j\}$ is valuable for planning purposes, whether in the private (retail) sector or for public facilities such as hospitals and schools. This model is elaborated in section 4.3 as a basis for exploring the deployment of thermodynamic concepts in section 4.4. We can use what might be called phase 1 methods to estimate $\{S_{ij}\}$, but this shows the phase 2 task to be the modelling of the structural vector $\{W_j\}$. We indicate an approach to this in section 4.5.

We have already noted that it is appropriate to work through discrete zone systems. This means that for most modelling purposes, we are choosing a particular mathematical representation for space at the outset. It is possible in principle to work with a continuous space representation – and indeed many economists, for example, do so; but it is argued here that the discrete choice is a more effective base for modelling.

2.2. Adding the detail.

The archetypal models are invaluable for demonstrating the range of methods that can be brought to bear for the modelling task. We obviously recognise, however, that cities are much more complicated and huge progress has been made in adding the appropriate detail to these models (see, for example, Wilson. 1974, 2007-A, Bertuglia, Leonardi and Wilson, 1987). We should also recognise that there are other submodels that demand different formulations: for example, economic input-output models, flows of goods, even energy, leading to real thermodynamics! However, all that takes us beyond the immediate scope of the paper.

There are further complications to be added. A city as a system of interest is located in an environment and 'external' zones of some kind will be needed to incorporate all the relevant interactions. It is important to be able to produce results that are as independent as possible of choice of zoning system and associated boundaries. For the purposes of this paper, we will ignore these complications. However, we should note that it will be important to be able to consider an individual zone as a system of interest, with the rest of the city as its environment (see Wilson, 2008-B). We can apply a fruitful thermodynamic perspective to this notion.

3. Some key concepts of thermodynamics and statistical mechanics.

3.1. System descriptions and thermodynamic laws.

A system of interest will be described by variables that divide into two sets: the *extensive* variables, that are dependent on size, and the *intensive* variables that are system properties that are not size dependent. The volume of a gas, V, is an example of the first; its temperature, T, and pressure, P, are examples of the second. It is a task of thermodynamics analysis to seek state equations that relate the key variables. For an ideal gas, there is Boyle's Law:

$$PV = nRT \quad (1)$$

where n is a measure of the number of particles and R is a universal constant.

The two key laws of thermodynamics, the first and second, are concerned with (a) the conservation of energy and (b) the fact that a system's energy cannot be increased without an amount of work being done on the system which is greater than or equal to the energy gain. Longair's (1984, 2003) formulation of the first law is:

- energy is conserved if heat is taken into account.

For the second law, he cites two equivalent formulations due respectively to Clausius and Kelvin:

- no process is possible whose sole result is the transfer of heat from a colder to a hotter body (Clausius);
- no process is possible whose sole result is the complete conversion of heat into work (Kelvin).

There are a number of so-called thermodynamic functions of state and we briefly note each of them and their uses. The internal energy of the system is particularly important. It normally appears in differential form, for example as

$$dU = dQ + \Sigma_i X_i dx_i \qquad (2)$$

where dQ is the flow of heat and $\Sigma_i X_i dx_i$ represents the work done on the system by various external forces, $\{X_i\}$. The $\{x_i\}$ are system descriptors – variables – so that dx_i measures the change in the variable from the application of the force. Essentially, the increase in the internal energy is the sum of the heat flow in and the work done. We can introduce entropy, S, for the first time (in its thermodynamic form) by defining it through

$$dQ = TdS \qquad (3)$$

so that

$$dU = TdS + \Sigma_i X_i dx_i \qquad (4)$$

The second law can then be formulated as

$$TdS \geq 0 \qquad (5)$$

For a fluid, the descriptor is the volume, V, and the force is the pressure, P, so that the work done can be represented by PdV, and

$$dU = TdS - PdV \qquad (6)$$

There is a negative sign because the work done on the system produces a reduction in volume and so the minus sign turns this into a positive contribution to work. In other cases, the X and the x might be the degree of magnetisation brought about by a magnetic field, for example. The general formulation in equations (2) and (4) is particularly important for our discussion of cities in section 4 below: the challenge then is to identify the $\{X_i\}$ and the $\{x_i\}$ in that case.

We can introduce in turn, the free energy, F,

$$F = U - TS \qquad (7)$$

the enthalpy, H,

$$H = U + PV \qquad (8)$$

and the Gibbs function, G,

$$G = U - TS + PV = H - TS \qquad (9)$$

The differential forms are important. Using (5), we can see that

$$dF = -SdT - PdV \qquad (10)$$

For later, it is useful to derive dF in a more general form from equations (4) and (7):

$$dF = -Sdt + \Sigma_i X_i dx_i \qquad (10A)$$

$$dH = TdS + VdP \qquad (11)$$

$$dG = -SdT + VdP \qquad (12)$$

Each of these functions can be specified as a function of two variables and then all other properties can be deduced. So, as we have hinted, the trick is to choose the best function for a particular system of interest. The possibilities (again following Pippard) are: U(S, V), H(S, P), F(T, V) and G(T, P). We will see that the urban case favours the use equivalents of T and V and hence the free energy.

The free energy (Pippard,1957, p.56) is a measure - a decrease in F – of the work that can be done by a system in an isothermal reversible change. Given the second law, it is the *maximum* amount of work that can be done by a system. It is also the critical link between thermodynamics and statistical mechanics, as we will see shortly. We can also note that by inspection of equation (7), the principle of maximising entropy, which we will invoke below, is equivalent – other terms being kept constant – to minimising free energy. This notion has been very interesting exploited by Friston [for example – see Friston et al (2006) and Friston and Stephan (2007)] in a way that we will also examine briefly later in section 6.5.

The enthalpy is used in engineering and the Gibbs function, for example, in chemistry to handle varying numbers of particles – and mixtures. We will be interested below to explore the 'urban' roles for specific heats. These are the amount of heat that can be absorbed for a unit increase in temperature, either for a change at constant volume (C_V) or at constant pressure (C_P):

$$C_V = (\partial U/\partial T)_V$$
(13)

and

$$C_P = (\partial U/\partial T)_P + P(\partial V/\partial T)_P \quad (14)$$

3.2. Statistical mechanics: the Boltzmann picture.

The simplest Boltzmann model is represented by the microcanonical ensemble. This is a set of copies of the system each of which satisfies some constraint equations which describe our knowledge of the macro system. It is assumed that each copy can occur with equal probability but Boltzmann's great discovery was to show that one distribution occurs with overwhelming probability. This distribution can be found by maximising an appropriate probability function which then turns out to be, essentially, the entropy function[2]. For a perfect gas with a fixed number of articles, N and fixed energy, E, if n_i is the number of particles with energy ε_i, then the most probable number of particles in each energy level – the most probable distribution - is obtained by maximising the entropy:

$$S = -\Sigma_i n_i \log n_i \quad (15)$$

[2] The detailed justification for this is well known and not presented here.

subject to

$$\Sigma_i n_i = N \tag{16}$$

$$\Sigma_i n_i \varepsilon_i = E \tag{17}$$

to give

$$n_i = N\exp(-\beta\varepsilon_i)/ \Sigma_i \exp(-\beta\varepsilon_i) \tag{18}$$

where

$$\beta = 1/kT \tag{19}$$

T is the temperature and k is Boltzmann's constant.

It is convenient to define the partition function as

$$Z = \Sigma_i \exp(-\beta\varepsilon_i) \tag{20}$$

This analysis can be presented in terms of probabilities defined by

$$p_i = n_i/N \tag{21}$$

and the Shannon entropy

$$S = -\Sigma_i p_i \log p_i \tag{22}$$

It is at this point that we can introduce the link between thermodynamics and statistical mechanics through the free energy, F (and here we follow Finn, 1991). It can be shown that

$$F = - NkT\log Z \tag{23}$$

and all thermodynamic properties can be calculated from this. If we recall equation (10), we can immediately see that

$$S = (\partial F/\partial T)_V \tag{24}$$

and

$$P = - (\partial F/\partial V)_T \tag{25}$$

We can then see from equation (7) that

$$U = F - T(\partial F/\partial T)_V = -T^2[\partial/\partial T(F/V)] \quad (26)$$

If we work with equation (10A) instead of (10), we can see that

$$X_i = (\partial F/\partial x_i)_T \quad (27)$$

Suppose now that the energy can vary. The energy is most generally represented in a Hamiltonian formulation and so we denote it by H. We can now construct a canonical ensemble in which each element is a state of the system with potentially varying energy. For each 'system' energy, that part of the ensemble will be a copy of the corresponding microcanonical ensemble. That is, it can be shown (Wilson, 1970, Appendix 2) that the microcanonical distribution is reproduced in, that is in effect nested in, the canonical distribution for each energy value in the latter.

This time, we can again work with probabilities, but we denote them by P_r since they relate to the probability of the *system* state occurring – and we label a particular state r. We can then maximise a system entropy to get the result that:

$$P_r = \exp(-\beta H_r)/ \Sigma_r \exp(-\beta H_r) \quad (28)$$

If we then relax the remaining condition, on the number of particles, N, we can construct a grand canonical ensemble and carry through the same analysis leading to

$$P_r = \exp(-\mu N-\beta H_r)/ \Sigma_r \exp(-\mu N-\beta H_r) \quad (29)$$

where μ is to be interpreted as a chemical potential.

The partition functions in these cases are

$$Z = \Sigma_r \exp(-\beta H_r) \quad (30)$$

and

$$Z = \Sigma_r \exp(-\mu N-\beta H_r) \quad (31)$$

We will also be interested below to explore phase transitions – discrete changes in the system state. For first order changes, some derivatives of F will be indeterminate (and there will be latent heat); and for second order changes, this will be the case for second derivatives (and no latent heat). Phase transitions usually involve a change from an ordered to a less ordered state – or vice versa – and so are often characterised in terms of *order parameters*. It will be important to explore these for urban systems below.

3.3. Further systems of interest in statistical mechanics.

The brief summaries given so far are based on classical gases. We will see that for urban applications, people are distinguishable in the way that particles in a classical gas are distinguishable – there are no 'quantum' effects - and so this is appropriate. However, as indicated in the introduction, we will be interested to explore the concept of a classical Ising model in two dimensions. The Ising model deals with particles on a lattice. Locations in urban systems can be characterised by grids and urban structure can then be thought of as structure at points on a lattice. (In practice, it is likely to be more complicated than this, but topologically an urban structure can almost certainly be transformed into a lattice and so the analogy can be pursued.)

The Ising model is concerned with spin systems and the alignment of spins at certain temperatures that produce magnetic fields. In the case of the one-dimensional Ising model with only neighbour-to-neighbour interaction, and spins σ_i at each lattice point, i, then the Hamiltonian is

$$H = -J\Sigma_{ij}\ \sigma_i\ .\sigma_j \qquad (32)$$

where J measures the strength of the interaction and the probability of a particular configuration occurring (using r now to label states) is again

$$P_r = \exp(-\beta H_r) / \ \Sigma_r \ \exp(-\beta H_r) \qquad (33)$$

but for the Hamiltonian defined in (32). We will explore below a generalised version of this model for urban structures and we will be particularly interested in modelling phase transitions which, in the urban case, involve shifts to new kinds of structure.

4. The thermodynamics of the city

4.1. Introduction.

In this section, we combine presentations of some archetypal models of cities which have been, or can be, rooted in concepts that are in common with those of statistical mechanics – representing transport flows, flows to retail centres and the evolution of retail centre structure. We intersperse these presentations with explorations of thermodynamic and statistical mechanical analogies.

In section 4.2, we present the transport model and in 4.3, the model of flows to retail centres. The thermodynamics of these spatial interaction systems is then explored in section 4.4. In section 4.5, we proceed to models of the evolution of urban structure, again using retail as an example and the thermodynamics of this model are explored in section 4.6. In 4.7, we present an alternative – entropy-maximising - model of urban structure and the associated thermodynamics.

4.2. The transport model.

Transport flows were initially modelled on the basis of an analogy with Newtonian physics – the so-called gravity model. We use the notation introduced in section 2.

$$T_{ij} = KO_iD_jc_{ij}^{-\beta} \quad (34)$$

This proved unsatisfactory and various factors were added to improve the fit to reality. The breakthrough (Wilson, 1967) was to recognise that these had a the resemblance to statistical mechanics' partition functions. It is then possible to use a version of the microcanonical ensemble presented earlier, but instead of a single state label, i, there is a double label, (i ,j). The constraint equations then become

$$\Sigma_j T_{ij} = Oi \quad (35)$$

$$\Sigma_i T_{ij} = D_j \quad (36)$$

$$\Sigma_i T_{ij}c_{ij} = C \quad (37)$$

C is the urban equivalent of 'energy' for this system. If c_{ij} is measured in money units, then C is measured in money units also. The 'number of particles' constraint – a single equation in physics – is replaced by the set of constraints (35) and (36). Then, maximising a suitable 'entropy'[3]

[3] There are many possible definitions of entropy that can be used here, but for present purposes, they can all be considered to be equivalent.

$$S = -\Sigma_i T_{ij} \log T_{ij} \quad (38)$$

gives, subject to (34)-(36), the so-called doubly-constrained model:

$$T_{ij} = A_i B_j O_i D_j \exp(-\beta c_{ij}) \quad (39)$$

Recall that $\{c_{ij}\}$ represents a measure of the cost of travel from i to j. The parameter β measures the 'strength' of the impedance. It can be determined from (37) if C is known, but in practice it is likely to be treated as a parameter of a statistical model and estimated from data. A_i and B_j are balancing factors to ensure that (35) and (36) are satisfied. Hence

$$A_i = 1/\Sigma_j B_j D_j \exp(-\beta c_{ij}) \quad (40)$$

and

$$B_j = 1/\Sigma_i A_i O_i \exp(-\beta c_{ij}) \quad (41)$$

The inverses of A_i and B_j are the analogues of the partition functions. However, they do not translate easily (or at all) into thermodynamic form. As noted earlier, equations (35) and (36) are the transport equivalent of (16), but we now have 2N equations rather than one (where N is the number of zones).[4]

4.3. Retail systems: interaction models as location models.

The next step is to introduce a spatial interaction model that also functions as a location model. We do this through the singly-constrained 'retail' model that is, retaining a constraint analogous to (35), but dropping (36). We begin with the conventional model and introduce a new notation to distinguish it from the transport model. Again we use the notation introduced in section 2: S_{ij} is the flow of spending power from residents of i to shops in j; e_i spending per head and P_i the population of i. W_j is a measure of the attractiveness of shops in j. α and β are parameters – the Lagrangian multipliers associated with the appropriate constraints.

[4]Can we take $A_i B_j$ as an i-j partition function? Can we work backwards and ask what we would like the free energy be for this system? If equation (37) specifies the energy and β (=1/kT) the temperature, then F = U – TS becomes F = C – S/kβ? Then if F = NkT logZ, what is Z?

The vector $\{W_j\}$ can then be taken as a representation of urban structure – the configuration of W_js. If many W_js are non-zero, then this represents a dispersed system. At the other extreme, if only one is non-zero, then that is a very centralised system. (Later, we will construct an 'order parameter' from the $\{W_j\}$ array in our exploration of possible phase transitions.) A spatial interaction model can be built for the flows on the same basis as the transport model. Then, maximising an entropy function:

$$-\Sigma_{ij} S_{ij} \log S_{ij} \quad (42)$$

we find

$$S_{ij} = A_i e_i P_i W_j^{\alpha} \exp(-\beta c_{ij}) \quad (43)$$

where

$$A_i = 1/ \Sigma_k W_k^{\alpha} \exp(-\beta c_{ik}) \quad (44)$$

to ensure that

$$\Sigma_j S_{ij} = e_i P_i \quad (45)$$

$$\Sigma_{ij} S_{ij} \log W_j = X$$
(46)

and

$$\Sigma_{ij} S_{ij} c_{ij} = C \quad (47)$$

Equation (46) represents a new kind of constraint: $\log W_j$ is a measure of size benefits to consumers at j and X an estimate of the total. α is a parameter associated with how consumers value 'size' of retail centres – and is actually the Lagrangian multiplier that goes with the constraint (46). As in the transport model, C is the total expenditure on travel. β measures travel impedance as in the transport model and is the Lagrangian multiplier that associated with (47).

Because the matrix is only constrained the origin end, we can calculate the total flows into destinations as

$$D_j = \Sigma_i S_{ij} = \Sigma_i e_i P_i W_j \exp(-\beta c_{ij})/ \Sigma_k W_k \exp(-\beta c_{ik})$$
(48)

and this is how the model also functions as a location model[5].

4.2. The thermodynamics of spatial interaction systems.

We begin with the transport model. It is clear from a comparison of equations (14)-(17) on the one hand and equations (33)-(39) on the other that the transport model is essentially based on a microcanonical ensemble with double labels (i, j) for 'energy' states instead of the single i-labels in the classical gas model. This leads to the conclusion, already noted above, that C can be taken to represent total 'energy' in some sense and the c_{ij}s, individual energy states. c_{ij} is a measure of impedance, some kind of transport cost. If there were contributions of an opposite sign, the cost might be interpreted as 'utility' and we will see such an example shortly. It is generally recognised that to make the models work, c_{ij} should be taken as a generalised cost, a weighted sum of elements like travel time and money cost. To take the thermodynamic analogy further, we do need a unit and, to fix ideas, we will take 'money' as that unit. These will then be the units of 'energy' in the system. (For simplicity, we will henceforth drop the quotation marks and let them be understood when concepts are being used through analogies.) Given that the units are defined, then the β parameter (in either the transport or the retail flow model), and the definition of a suitable Boltzmann constant, k, will enable us to define temperature through

$$\beta = 1/kT \tag{49}$$

We are accustomed to estimating β through model calibration. *An interesting question is how we define k as a 'universal urban constant' which would then enable us to estimate the 'transport temperature' of a city.* Note that if c_{ij} has the dimensions of money, then β has the dimensions of $(\text{money})^{-1}$, then from (41), kT would have the dimensions of money. If k is to be a universal constant, then T would have the dimensions of money. It is also interesting to note that it has been proved that (Evans, 1973), in the transport model, as $\beta \to \infty$, the array $\{T_{ij}\}$ tends to the solution of the transportation problem of linear programming in which case C, in equation (36), tends to a minimum. This is the thermodynamic equivalent of the temperature tending to absolute zero and the energy tending to a minimum.

[5] This model, in more detailed form, has been widely and successfully applied.

In the case of the retail model, it is now convenient to note that W_j^{α} can be written

$$W_j^{\alpha} = \exp(\alpha \log W_j) \quad (50)$$

If we then assume, for simplicity and for illustration, W_j can be taken as 'size' and that benefits are proportional to size, then the term $\alpha \log W_k$ is the promised example of a positive contribution to energy. It shows explicitly that $\log W_j$ can be taken as a measure of the utility of an individual going to a shopping centre of size W_j but at a transport cost, or disutility, represented by c_{ik}. The significance of this in the thermodynamic context is that α can be seen (via another Boltzmann constant, k′) as a different kind of temperature, T′:

$$\alpha = 1/ k'T' \quad (51)$$

It was originally shown in Wilson (1970), following Jaynes (1957), that this argument can be generalised to any number of constraints and hence any number of temperatures. It can easily be shown, as in Physics, that if two systems are brought together with different temperatures, then they will move to an equilibrium position at an intermediate temperature through flows of heat from the hotter to the colder body. This also means, therefore, that in this case, there can be flows of different kinds of heat. In this case, the flow of heat means that more people 'choose' destinations in the 'cooler' region.

In order to take the argument and the analogy further, we need to recognise two kinds of change through work being done on the system (or heat flowing). In terms of the transport elements of either model, this can be a δC change or a δc_{ij} change. The former is a whole system change that means, for example, there is a greater resource available for individuals to spend on transport – and this will decrease β and hence increase the temperature; the latter would probably be produced by a network change – say the investment in a new link. Even with fixed C, if this leads to a reduction in cost, we would expect it to generate an increase in temperature. In terms of the physics analogy, a positive δC change is equivalent to an increase in energy and it would be possible in principle to define an external coordinate, x_i, and a generalised force, X_i, so that $X_i \delta x_i$ generated δC. It is less easy to find a physics analogue for δc_{ij} changes – because that would involve changing energy levels.

This analysis enables us to interpret the principal laws of thermodynamics in this context. 'Work done' on the system will be manifested through either δC or δc_{ij} changes. Essentially, what the laws tell us is that there will be some 'waste' through the equivalent of heat loss. Note that an equivalent analysis could be offered for the retail model for δW_j or δX changes.

We should now return to the basics of the thermodynamic analogy and see if there are further gains to be achieved – particularly by returning to the $\Sigma_i X_i dx_i$ terms [from equation (2)]. We have available to us a temperature through the parameter β (actually 1/kT, an inverse temperature).

A first step is to explore whether there is an x_i which is the equivalent of a volume, V. The volume of a gas is the size of the container. In this case, for simplicity for this initial exploration, we can take the area, A, of the city as a measure of size[6]. This would then allow us to work with the free energy as a function of T and V – in the urban case, β and A: F(β, A), say. We can then explore the idea of a state equation and it seems reasonable to start with Boyle's law since people in cities are being modelled on the same basis as an ideal classical gas. This suggests, by analogy with equation (1) that:

$$PA = NRT \tag{52}$$

where N is the total population and R is a constant. In terms of β, this becomes

$$P = NR/\beta kA \tag{53}$$

where we have taken A to the other side of the equation[7]. There are, of course, two constants, R and k, in this equation which cannot be obtained in the same way as in Physics, but let us assume for the moment that they can be estimated. Then, equation (53) gives us a definition of an urban 'pressure'. It has the right properties intuitively: it increases if A or β decreases or N increases (in each case, other variables held constant).

We saw in the transport case that while we could find analogues of partition functions, the analogy was not exact. In the retail case we have dropped one set of 'number' constraints and this suggests that the inverse of the A_i term will function as a partition function. Consider

[6] We should explore whether we can determine a measure of A from the topology of the $\{c_{ij}\}$.

[7] Note that P appears to have the dimensions of 'density'x'money'.

$$Z_i = \Sigma_k \exp(\alpha \log W_k - \beta c_{ik}) \quad (54)$$

This looks like a partition function, but as a function for each zone i rather than for the system as a whole. This is because the consumers leaving a zone can be treated as an independent system[8]. It is perhaps then not too great a leap to make the heroic assumption that an appropriate partition function for the system is

$$Z = \Sigma_i Z_i = \Sigma_{ik} \exp(\alpha \log W_k - \beta c_{ik}) \quad (55)$$

We can then seek to work with the free energy and the model at equations (4) and (49). Then, using equation (22)

$$F = -[N/\beta]\log Z \quad (56)$$

We can also explore the standard method of calculating state functions from the free energy:

$$P = -(\partial F/\partial A)_T \quad (57)$$

$$S = -(\partial F/\partial T)_A \quad (58)$$

or, using (25)

$$S = -k\beta^2(\partial F/\partial \beta)_A \quad (59)$$

And, with U = C, using equation (23),

$$U = F - (\partial F/\partial T)_A = -T^2(\partial/\partial T.F/T)_A = \quad (\partial/\partial \beta.k\beta F)_A \quad (60)$$ [9]

In this formulation, A does not appear in the partition function. We might consider A to be defined by the topology of the $\{c_{ij}\}$ and possibly the spatial distribution of the W_j and this should be explored further. Indeed, more generally we might write equation (57) as

$$X_i = -(\partial F/\partial x_i)_T \quad (61)$$

It might be particularly interesting to look at the concepts of specific heat. 'Heat' flowing into a city will be in the form of something like investment in the transport

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[8]ter Haar, Third |Edition p 202 does show that each subsystem within an ensemble can itself be treated as an ensemble provided there is a common β value

[9]What does this produce for U? And is it possible to do all the calculations implied by (55)-(59)?

system and this will increase T and hence decrease β but each city will have a specific heat and it will be interesting to look at how different cities can effectively absorb investment. This should connect to cost-benefit analysis, possibly through NPVs. We can build on equations (12) and (13):

$$C_V = (\partial U/\partial T)_V \quad \rightarrow -1/k\beta^2(\partial U/\partial \beta)_A$$
(62)

and

$$C_P = (\partial U/\partial T)_P + P(\partial V/\partial T)_P = [-1/k\beta^2(\partial U/\partial \beta)_P + P(\partial V/\partial \beta)_P] \qquad (63)$$

It remains a challenge to calculate these in the urban case.

We should also examine the possibility, noted earlier, of examining some of these concepts at the level of a zone within city – building on ter Haar's concept of subsystems.[10]

It remains to ask the question of whether there could be phase changes in spatial interaction systems? This seems intuitively unlikely for the spatial interaction models: smooth and fast shifts to a new equilibrium following any change is the likely outcome. If the model is made more realistic – and more complicated – by adding different transport modes, then the position could be different. There could then be phase changes that result in a major switch between modes at some critical parameter values. (See, for example, Wilson, 1976.) However, there is the possibility of significant phase changes in the structural model and it is to this that we now turn.

4.5. A model of urban structure and its evolution.

We have presented an archetypal singly-constrained spatial interaction model, representing (among other things) flows to the retail sector. We can now add a suitable hypothesis for representing the dynamics (following Harris and Wilson, 1978):

$$dW_j/dt = \varepsilon (D_j - KW_j)W_j$$
(64)

where K is a constant such that KW_j can be taken as the (notional) cost of running the shopping centre in j[11]. This equation then says that if the centre at j is profitable,

[10] It is possible to introduce a β_i rather than a β which reinforces this idea.

it grows; if not, it declines. The parameter ε determines the speed of response to these signals.

The equilibrium position is given by

$$D_j = KW_j \quad (65)$$

which can be written out in full, using equation (48), as

$$\Sigma i\{e_i P_i W_j \exp(-\beta c_{ij})/\Sigma_k W_k \exp(-\beta c_{ik})\} = KW_j \quad (66)$$

and these are clearly nonlinear simultaneous equations in the $\{W_j\}$.

The equations (64) are analogous to Lotka-Volterra equations – in the form of species competing for resources. In this case, we have retail developers competing for consumers. Because this model combines Boltzmann's statistical mechanics (B) and Lotka's and Volterra's dynamics (LV), these have been characterised as BLV models and it has been shown that they have a wide range of application (Wilson, 2007-B).

What is clear to the present time is that it is possible to characterise the kinds of configurations that can arise for different regions of α and β space: for larger α and lower β, there are a smaller number of larger centres; and vice versa[12]. This can be interpreted to an extent for a particular zone, say j, by fixing all the W_k, for k not equal to j. A key challenge is to solve this problem with all the W_js varying simultaneously. There are many procedures for solving the equations (49) iteratively but we constantly need to bear in mind the sensitivity to the initial conditions – the path dependence – and the possibility of multiple solutions. What we might learn from a statistical mechanics formulation is whether among the multiple solutions, there is one that is very much the most probable.

The zonal interpretation is shown in Figure 1. The left and right hand sides of equation (65) are plotted separately and of course, the intersections are the possible equilibrium points. If $\alpha \leq 1$, there is always a possible equilibrium point, but if $\alpha > 1$, there are three possible cases: only zero as an equilibrium; one additional non-zero stable state; and the limiting case that joins the two. The β value also determines the

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[11] K could be j-dependent as K_j (and indeed, usually would be) but we retain K for simplicity of illustration.

[12] Clarke and Wilson (1985), Wilson (1984)

position of the equilibria. This analysis shows a number of properties that are typical of nonlinear dynamical systems: multiple (system) equilibria and strong path dependence – that is, sensitive dependence on initial conditions. It also shows that as the parameters α and β (and indeed any other exogenous variables) change slowly, there is the possibility of a sudden change in a zone's state – from development being possible to development not being possible, or vice versa [as depicted by the two KW_j lines in Figure 1 (b) and (c)]. These kinds of change can be characterised as phase transitions – in this case at a zonal level, but clear there will be system wide changes of this kind as well. It will turn out that there is the essence of a very powerful tool here for identifying complex phase transitions. We return to this in the section 4.6.

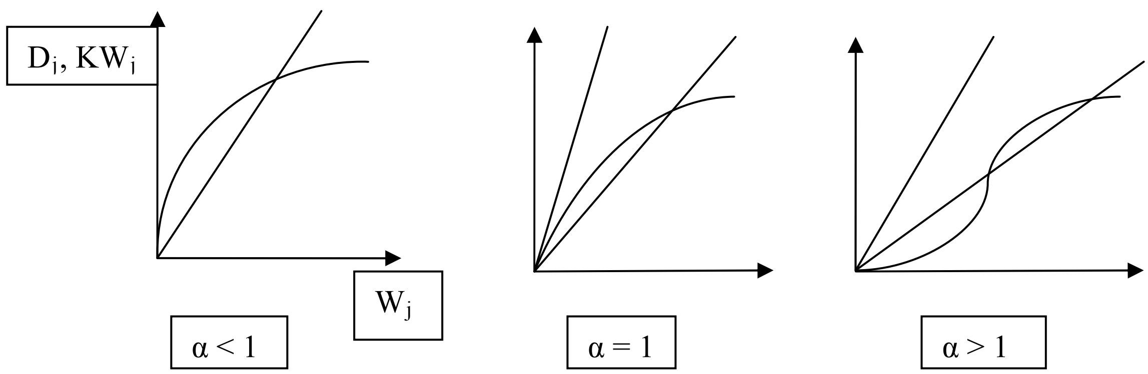

Figure 1. (a) (b) (c)

Recall that this analysis is dependent, for a particular W_j, on the set $\{W_k\}$, $k \neq j$, being constant. It is almost certainly a good enough approximation to offer insight, but the challenge is to address the problem of simultaneous variation. The system problem is to predict equilibrium values for the whole set $\{W_j\}$ and the trajectories through time, recognising the points at which phase changes take place. This is where newer statistical mechanics models potentially can help as we will see in the section 4.5 below. This analysis does, however, indicate phase changes, and below, we will explore the derivatives of F to look for indeterminacy.

4.4. The thermodynamics of structural change.

We have seen that the spatial interaction model, whether in its doubly-constrained (transport) form, $\{T_{ij}\}$, or singly-constrained (retail) form, $\{S_{ij}\}$, is best represented by a microcanonical ensemble and we can reasonably assume a rapid return to equilibrium following any change. We have offered an equation representing the dynamics of $\{W_j\}$ evolution but we can now work towards an interpretation of this model in a statistical mechanics format. It will be represented by a canonical ensemble and the return to equilibrium is likely to be much slower: it takes developers much longer to build a new centre than for individuals to adjust their transport routes for example. What is more, the two systems are linked because the structural variables $\{W_j\}$ are exogenous variables in the retail model (and there is an equivalent vector in the transport model). In the case of the structural model, we will have to assume some kind of steady state independent rapid-return-to-equilibrium for the interaction arrays. We have indicated in the previous section that there will be discrete changes. We now explore the possible statistical mechanics' bases to see if these are in fact phase changes.

In section 3.3, we introduced the one-dimension Ising model. Equations (30) and (31) are repeated here for convenience:

$$H = -J\Sigma_{ij}\, \sigma_i\, .\sigma_j \qquad (30A)$$

$$P_r = \exp(-\beta H_r)/\, \Sigma_r\, \exp(-\beta H_r) \qquad (31A)$$

The interactions in the Ising model are only with nearest neighbours and there are no phase transitions. However, when it is extended to two and three dimensions, there are phase transitions, but it is very much more difficult to solve. In our case, of course, we are interested in interactions that extend, in principle, between all pairs. Such models have been explored in statistical mechanics and, below, we explore them and seek to learn from them – cf. Martin (1991).

We can consider zone labels i and j to be represented by their centroids which can then be considered as the nodes of a lattice. The task, then, is to find a Hamiltonian, H_r, as a function of the structural vector $\{W_j\}$. We can then write (31A) as

$$P_r=\exp(-\beta H_r(\{W_j\}))/\Sigma_r\exp(-\beta H_r(\{W_j\}) \qquad (67)$$

and we have to find the $\{W_j\}$ that maximises P_r. Since the denominator is the same for each r, this problem becomes

$$L[\{W_j^{opt}\}] = \text{Max}_r \exp(-\beta H_r(\{W_j\})) \quad (68)$$

So the immediate issue is to decide on the Hamiltonian. Suppose we take the measure of profit used in equation (63). Then

$$H = \Sigma_j(D_j - KW_j) \quad (69)$$

and the problem becomes

$$L[\{W_j^{opt}\}] = \text{Max}_r \exp[-\beta\Sigma_j(D_j - KW_j)] \quad (70)$$

where K is a unit cost for retailers and D_j can be obtained from equations (65) and (50); substitution then gives

$$L[\{W_j^{opt}\}] = \text{Max}_r \exp[-\beta\Sigma_j(\Sigma_i\{e_iP_iW_j\exp(-\beta c_{ij})/\Sigma_kW_k\exp(-\beta c_{ik})\} - KW_j)] \quad (71)$$

which shows what a formidable problem this appears to be. However, scrutiny of the right hand side shows that we maximise L by maximising the exponent and because of the first negative sign, this is achieved by minimising

$$\Sigma_j(\Sigma_i\{e_iP_iW_j\exp(-\beta c_{ij})/\Sigma_kW_k\exp(-\beta c_{ik})\} - KW_j) \quad (72)$$

which then suggests that the equilibrium value for $\{W_j\}$ occurs when this expression is a minimum. However, by inspection, we can see that this happens when each term within Σ_j is zero:

$$\Sigma_i\{e_iP_iW_j\exp(-\beta c_{ij})/\Sigma_kW_k\exp(-\beta c_{ik})\}= KW_j \quad (73)$$

which is, of course, simply the equilibrium condition (65) [or (66)]. This then seems to indicate that a statistical mechanics exposition produces an equivalent equilibrium condition for the $\{W_j\}$.

What we know from the analysis of Figure 1 is that at a zonal level, there are critical values of α and β, for example, beyond which only $W_j = 0$ is a stable solution for that zone – that is, the expression inside Σ_j. So we know that there are critical points at a zonal level at which, for example, there can be a jump from a finite W_j to a zero W_j. (See Dearden and Wilson, 2008, for a simulation of this.)This implies there is a set of α and β at which there will be critical changes somewhere in the system. This is particularly interesting when we compare this situation to that in statistical mechanics. There, we are usually looking for critical temperatures for the whole system at which there is a phase transition. Here, there will be many more system phase transitions, but in each case consisting of a zonal transition (which then affects the system as a whole – since if a W_j jumps to zero, then other W_ks will jump upwards – or vice versa). It would be interesting to see whether the set of critical αs and βs form a continuous curve. If we further add, say, K and the $\{e_iP_i\}$, then we are looking for a many-dimensional surface. It will also be interesting to see whether there are other systems – ecosystems? – that exhibit this kind of phase change.

To take the argument further at the system level, we need to construct an order parameter. In Physics, at a phase change, there is a discontinuity in the order parameter and hence indeterminacy in some derivatives of the free energy. An obvious example in Physics is in magnetism: an ordered system has particles with spins aligned – ordered – and there can be phase transitions to and from disordered states. In these cases, the order parameters are straightforward to define. In the urban case, intuition suggests that it is the nature of the configurations of $\{W_j\}$ that we are concerned with. A dispersed system with many small centres can be considered less ordered than one with a small number of large centres. This suggests that we should examine $N[W_j>x]$ – the number of W_j greater than some parameter x. If x is set to zero, this will be a measure of ubiquity of centres and we know that there will be transitions at $\alpha = 1$. Or we could set x to be large and seek to identify configurations with a small number of large centres to see whether they are achieved through phase transitions as parameters vary or continuously[13] - see Wilson (2008-D).

4.7. An alternative thermodynamic formulation for the $\{W_j\}$

In this analysis so far, we have assumed that $\{W_j\}$ can be obtained by solving the equilibrium equations [(61), (62) or (69)]. It is interesting to explore the possibility of a suboptimal $\{W_j\}$ via entropy maximising – something more like a lattice model with each W_j as an occupation number.. We can use the same argument that generates conventional spatial interaction models and differentiates

[13]It would be interesting to calculate the derivatives of the free energy – the F-derivatives - to see whether there is a way of constructing $N[W_j>x]$ out of F. Are we looking at first or second order phase transitions?

them from the transportation problem of linear programming. (And, of course, as we noted earlier, it has been shown that as $\beta \rightarrow \infty$, the s.i. model solution tends to the linear programming limit.) We can proceed as follows. Assume $\{S_{ij}\}$ is given[14]. Then maximise an entropy function in $\{W_j\}$ subject to appropriate constraints.

$$\text{Max } S = - \sum_j W_j \log W_j$$
(74)

such that

$$\sum_{ij} S_{ij} \log W_j = X$$
(75)

and

$$\sum_i S_{ij} = kW_j + Y \qquad (76)$$

X and Y are constants – X determining the total amount of benefit that consumers derive from size (or attractiveness) and Y the extent to which the equilibrium condition (A1.1) is being treated as suboptimal. The Lagrangian for this problem is

$$L = -\sum_j W_j \log W_j - \mu \sum_i [S_{ij} - KW_j - Y] - \alpha(\sum_i S_{ij})/W_j \qquad (77)$$

and setting

$$\partial L/\partial Wj = 0 \qquad (78)$$

gives, with some re-arrangement

$$\log W_j + \alpha D_j/W_j = \mu K_j$$
(79)

(where we have substituted D_j for $\sum_i S_{ij}$ without loss of generality since we are taking the $\{S_{ij}\}$ as fixed.) These equations could be solved numerically for {Wj} – and indeed graphically – see Wilson (2008-E).

It is then interesting to interpret equation (79) and then to look at the $\alpha \rightarrow \infty$ limit. Write (79), by dividing by μ, as follows:

$$(1/\mu)\log W_j + \alpha D_j/\mu W_j = K_j \qquad (80)$$

[14] It can be shown that we can carry out an entropy maximising calculation on $\{S_{ij}\}$ simultaneously and that leads to a conventional s.i. model and the same model for $\{W_j\}$. The implication of this argument is that if we obtain a $\{W_j\}$ model with the method given here, we should then recalculate $\{S_{ij}\}$ from an s.i. model and then iterate with $\{W_j\}$.

The right hand side is clearly cost per square foot. The first term on the right hand side is a measure of scale benefits; the second term is revenue per square foot modified by the factor α/μ.

By analogy with the linear programming version of the transport model, as $\alpha \to \infty$, we would expect the normal equilibrium condition to be satisfied and hence $Y \to 0$. Equation (79) then suggests that as $\alpha \to \infty$, we must have $\mu \to \infty$ in such a way that $\alpha/\mu \to 1$. The first term in (79) then clearly tends to 0 and the equation then becomes equivalent to (72).

5. Ongoing challenges.

5.1. Introduction.

We noted at the outset that there have been three phases of relevant work in urban science:

- spatial interaction models – and associated location models - rooted in statistical mechanics, which work very effectively;
- models of developing and evolving structures, including the recognition of urban phase transitions;
- the use of newer methods in statistical mechanics to accelerate our understanding of development and evolution

Within this framework, we have aimed to add thermodynamic interpretations to the findings of each phase – an area that has been raised in the past but far from fully developed. How do we now move forward?

5.2. Spatial interaction.

These are the models about which we can feel most confident in practice. Only archetypal models have been presented here, but by now they have been fully disaggregated and tested in a wide variety of circumstances. However, it is clear from the argument presented here that there remain possibly interesting areas of interpretation which can be developed through the thermodynamic analogy. In particular, it would be valuable to seek an understanding of the urban partition functions that arise from the more complex 'particle number' constraints that are introduced. There is also scope for a fuller exposition of the thermodynamics of these models. A start has been made in this paper but it would be useful, for example, to expound more fully the external variables that underpin changes in these systems.

5.3. Development and evolution.

These issues have only been explored to date with archetypal models. There is a case for exploring, for example, phase transitions with more realistic disaggregated models and also exploring (in the case of the retail model) alternative revenue and production (i.e. cost) functions to see whether new kinds of phase transitions would emerge. Again, there is a need fully to articulate the thermodynamics. It is also clear that the kinds of phase transitions that are now evident in the archetypal models have not been fully explored and that new powerful methods of computer visualisation will facilitate this.

5.4. The 'new' thermodynamics and statistical mechanics.

We noted at the outset that authors such as Ruelle (2004)and Beck and Schlogel (1993) – and many others - are presenting the mathematics of thermodynamics and statistical mechanics in a more general format and demonstrating in principle the applicability to a wider range of systems. It would be valuable systematically to translate the models presented in this paper into these formats to explore the extent to which further advances are possible. We have only scratched the surface of possibilities in this paper and further research is to be encouraged.

5.5. Models in planning.

Urban models have long had uses in various forms of planning – public and commercial – through their forecasting capabilities and, to a lesser extent, through being embedded in optimisation frameworks. Our understanding of nonlinearities now puts a bound in forecasting capabilities but in an interesting way. While forecasting may be impossible in terms of structural variables over a long time scale – because of path dependence and phase transitions – what becomes possible is the identification of phase transitions that may be desirable or undesirable and then one aspect of planning is to take actions to encourage or avoid these as appropriate.

There is a potential new interest, that we have alluded to briefly earlier, which brings statistical mechanics to bear on urban planning, and that is Friston's (el al's) work on free energy and the brain. It is interesting to place this model into a planning framework (Wilson, 2008-F). The essence of Friston's argument – for the purposes of building the analogy – is to model the brain and its environment as interacting systems, and that the brain, through its sense mechanisms, builds a model of the environment and that it handles environmental uncertainties through free energy minimisation. If the brain is replaced by 'urban planning system' and its environment by 'the city', then Friston's argument resonates with Ashby's (1956) law of requisite variety – essentially in this case that the planning system has to model the city in order to have a chance of success.

5.6. Concluding comments.

There have been some spectacular successes in the application of statistical mechanics to urban modelling and some insights have been achieved in adding thermodynamic interpretations. However, it is also clear that the potential benefits of combining the tools from different disciplines in the urban modelling context have not been fully worked out. What is needed is a coming together of skills, the building of new interdisciplinary teams: urban modellers, statistical physicists and the mathematicians who have been generalising the thermodynamic and statistical mechanics formalisms. It might also be valuable to add the skills of those who have been using these tools for modelling in other fields, such as neuroscience. In some cases, neuroscience being an example, the emphasis has been on talking a statistical (Bayesian) view and this complements the mathematical one in an interesting way. It may be helpful to conclude, therefore, with some indications of what remains to be achieved – but which intuition suggests is achievable!

The urban 'big picture' needs to be completed – for example through the specification of suitable 'external variables' and generalised forces – the $X_i\delta x_i$ terms – for cities. We perhaps made the beginnings of progress by introducing 'area' as a quasi 'volume' measure but leaving open the question of whether a better measure could be found from $\{c_{ij}\}$ topology. We also had some difficulty in specifying 'urban' partition functions because of the usual nature of the 'number of particles'/origin-destination constraints. This is a research question to be resolved.

Potentially the biggest advances to come lie in the modelling of the evolution and emergence of structures – the {Wj} in the archetypal model. Again, intuition suggests that the methods down being applied to solids in statistical physics – and their mathematical generalisations, should enable us to make more progress than we have achieved so far. However, that progress is not inconsiderable: it has allowed us to identify phase transitions in urban evolution and to show that they are of a different character to the most obvious ones in physics.

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