Chapter 2
The "Thermodynamics" of the City

Evolution and Complexity Science in Urban Modelling

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2.1 Introduction

The primary objectives of this chapter are twofold: first, to offer a review of progress in urban modelling using the methods of statistical mechanics; and second, to explore the possibility of using the *thermodynamic* analogy in addition to statistical mechanics. 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. *We will show that these methods of statistical mechanics and thermodynamics illustrate the contribution of urban modelling to complexity science and form the basis for understanding the evolution of urban structure.*

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. Examples of these broader approaches are provided by Beck and Schlagel (1993) and Ruelle (1978, 2004). The recognition of the power of the method and its wider application goes back at least to the 1950s (Jaynes, 1957, for example) but understanding its role in complexity science is much more recent. However, these methods are now being seen as offering a major contribution. In general, the applications have mainly been in fields closely related to the physical sciences. The purpose of this chapter 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. The urban modelling field can be seen, in its early manifestation, as a precursor of complexity science; and, increasingly, as an important application within it (Wilson 2000).

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There have been two main phases of development in this branch of 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 flows 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 fields such as developmental biology. It is a powerful example of the possibility of modelling evolution within complexity science.

The emerging third phase reconnects with statistical mechanics. It was shown in the evolution modelling that there could be sudden changes in structure at critical values of parameters. Are these analogues of phase transitions in statistical mechanics? There was always the possibility that analogies with Ising models in Physics and their progeny – concerned with the properties of molecules on a lattice – would offer further insights since these represented a kind of locational structure problem and some interesting mathematics were associated with these models. Statistical mechanics is now handling much more complex structural models and there is a much fuller understanding of phase transitions. This makes it worthwhile to pursue the analogy again.

The chapter is structured as follows. In Sect. 2.2 we present two archetypal models – first the transport model and second the retail model – to represent urban systems of interest. In each case, we combine the description of the models with a thermodynamic interpretation. In Sect. 2.3, we show how the retail model can be extended to be an archetypal model of the evolution of urban structure and, again, the associated thermodynamics. In Sect. 2.4, we explore future challenges.

2.2 The Thermodynamics of Spatial Interaction

2.2.1 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 and flows to retail centres. We intersperse these presentations with explorations of thermodynamic and statistical mechanical analogies. In Sect. 2.2.2, we introduce the systems of interest and define the key variables. In Sect. 2.2.3, we present the transport model and in Sect. 2.2.4, the model of flows to retail centres.

2.2.2 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 Sect. 2.2.3.

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 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 Sect. 2.2.4. 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 dynamics of the structural vector $\{W_j\}$. We indicate an approach to this in Sect. 2.3.

2.2.3 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 Sect. 2.2.2.

$$T_{ij} = KO_iD_jc_{ij}^{-\beta}, \tag{2.1}$$

where k and β are constants. 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 resemblance to statistical mechanics' partition functions.

To show the connection and to facilitate later analysis, we introduce some of the core concepts of statistical mechanics here. 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.[1] 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:

$$S = -\Sigma_i n_i \log n_i, \tag{2.2}$$

subject to

$$\Sigma_i n_i = N, \tag{2.3}$$

$$\Sigma_i n_i \varepsilon_i = E, \tag{2.4}$$

to give

$$n_i = N \exp(-\beta\varepsilon_i)/\Sigma_i \exp(-\beta\varepsilon_i), \tag{2.5}$$

where

$$\beta = 1/kT. \tag{2.6}$$

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

It is convenient to define the partition function as:

$$Z = \Sigma_i \exp(-\beta\varepsilon_i). \tag{2.7}$$

It is useful for a future point in the argument to note here that we can link thermodynamics and statistical mechanics through the free energy, F (and here we follow Finn 1993) defined in terms of the partition function as:

$$F = -NkT \log Z, \tag{2.8}$$

and all thermodynamic properties can be calculated from this.

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

The post-Newton, Boltzmann-like, transport model can then be developed on the basis of such a microcanonical ensemble. Now, instead of a single state label, i, representing energy levels, there is a double index, (i,j), labelling origin–destination pairs. The constraint equations then become:

$$\Sigma_j T_{ij} = O_i, \tag{2.9}$$

$$\Sigma_i T_{ij} = D_j, \tag{2.10}$$

$$\Sigma_i T_{ij} c_{ij} = C. \tag{2.11}$$

The "number of particles" constraint – a single equation in physics – is replaced by the sets of constraints (2.9) and (2.10). C is clearly the urban equivalent of "energy" for this system and the c_{ij}, measures of the cost of travel from i to j, are the equivalent of energy levels. If c_{ij} is measured in money units, then C is measured in money units also. Then, maximising a suitable "entropy"[2]

$$S = -\Sigma_i T_{ij} \log T_{ij} \tag{2.12}$$

gives, subject to (2.9)–(2.11), the so-called doubly-constrained model:

$$T_{ij} = A_i B_j O_i D_j \exp(-\beta c_{ij}). \tag{2.13}$$

The parameter β measures the "strength" of the impedance: if β is large, trips are relatively short, and vice versa. It can be determined from (2.11) 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 (2.9) and (2.10) are satisfied. Hence:

$$A_i = 1/\Sigma_j B_j D_j \exp(-\beta c_{ij}), \tag{2.14}$$

and

$$B_j = 1/\Sigma_i A_i O_i \exp(-\beta c_{ij}). \tag{2.15}$$

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.

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

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

take the thermodynamic analogy further, we do need a common unit and, as noted earlier and to fix ideas, we take "money" as that unit. These will then be the units of "energy" in the system.[3] Given that the units are defined, then the β parameter, together with the definition of a suitable Boltzmann constant, k, will enable us to define temperature through:

$$\beta = 1/kT. \tag{2.16}$$

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 with c_{ij} having the dimensions of money, then β has the dimensions of $(\text{money})^{-1}$ and so from (2.16), 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 (2.11), tends to a minimum. This is the thermodynamic equivalent of the temperature tending to absolute zero and the energy tending to a minimum.

2.2.4 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 (2.9), but dropping (2.10). We begin with the conventional model and introduce a new notation to distinguish it from the transport model. We use the notation introduced in Sect. 2.2.2

The vector $\{W_j\}$ can 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. A spatial interaction model can be built for the flows on the same basis as the transport model. Maximizing an entropy function:

$$-\Sigma_{ij} S_{ij} \log S_{ij}, \tag{2.17}$$

we find

$$S_{ij} = A_i e_i P_i W_j^{\alpha} \exp(-\beta c_{ij}), \tag{2.18}$$

[3]For simplicity, we will henceforth drop the quotation marks and let them be understood when concepts are being used through analogies.

where

$$A_i = 1/\Sigma_k W_k^\alpha \exp(-\beta c_{ik}), \tag{2.19}$$

to ensure that

$$\Sigma_j S_{ij} = e_i P_i, \tag{2.20}$$

$$\Sigma_{ij} S_{ij} \log W_j = X, \tag{2.21}$$

and

$$\Sigma_{ij} S_{ij} c_{ij} = C. \tag{2.22}$$

Equation (2.21) represents a new kind of constraint. It is inserted to generate the W_j^α term in (2.18), but the form of this equation shows that log W_j can be taken as a measure of size benefits to consumers using 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 (2.21). In thermodynamic terms, as we will see shortly, X can be taken as another kind of energy. 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 (2.22).

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

$$D_j = \Sigma_i S_{ij} = \Sigma_i e_i P_i W_j^\alpha \exp(-\beta c_{ij})/\Sigma_k W_k^\alpha \exp(-\beta c_{ik}), \tag{2.23}$$

and this is how the model also functions as a location model.[4]

W_j^α can be written:

$$W_j^\alpha = \exp(\alpha \log W_j). \tag{2.24}$$

If we then assume, for simplicity and for illustration, W_j can be taken as "size" and that benefits are proportional to size, then this 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_{ij}. The significance of this in

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

the thermodynamic context is that α can be seen (via another Boltzmann constant, k') as related to a different kind of temperature, T':

$$\alpha = 1/k'T'. \tag{2.25}$$

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.

2.2.5 Deepening the Thermodynamic Analogy

In order to learn more from the thermodynamic analogy, we need to remind ourselves of some of the core concepts. 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.

There are a number of so-called thermodynamic functions of state and we briefly note those needed for our ongoing argument. The internal energy (which we will equate with our "C") is particularly important. It normally appears in differential form, for example as:

$$dU = dQ + \Sigma_i X_i dx_i, \tag{2.26}$$

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. For example, there may be a change in volume, V, an x-variable, from the application of pressure, P, an X-force.

We can introduce entropy, S, for the first time (in its thermodynamic form) by defining it through:

$$dQ = TdS, \tag{2.27}$$

so that

$$dU = TdS + \Sigma_i X_i dx_i. \tag{2.28}$$

The second law can then be formulated as:

$$TdS \geq 0 \tag{2.29}$$

(or, "entropy always increases"). For a fluid of volume, V, and pressure, P, the work done can be represented by PdV, and

$$dU = TdS - PdV \tag{2.30}$$

(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 (2.26) and (2.28) is particularly important for our discussion of cities below: the challenge then is to identify the $\{X_i\}$ and the $\{x_i\}$ in that case.

We can introduce the free energy, F, as:

$$F = U - TS, \tag{2.31}$$

and in differential form as:

$$dF = -SdT - PdV, \tag{2.32}$$

or in a more general form, from (2.28) and (2.31), as:

$$dF = -SdT + \Sigma_i X_i dx_i. \tag{2.33}$$

F can be specified as a function of T and V and then all other properties can be deduced.

The free energy (Pippard 1957, p. 56) is a measure of the work that can be done – a decrease in F – 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. We can also note that by inspection of (2.31), the principle of maximizing entropy, which we will invoke below, is equivalent – other terms being kept constant – to minimizing free energy. This notion has been very interestingly exploited by Friston [for example – see Friston et al. (2006) and Friston and Stephan (2007)] in a way that we will examine briefly later in Sect. 2.4.

In the case of spatial flow models, 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 of our archetypal models, 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. 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 (2.2)]. It is worth noting that a system of interest is 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:

$$PV = nRT, \tag{2.34}$$

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

In the urban case, we have available to us a temperature through the parameter β (actually $1/kT$, an inverse temperature). The next 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.[5] This would then allow us to work with the free energy as a function of T and V – or in the urban case, β and A: $F(\beta, A)$, 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 (2.34) that:

$$PA = NRT, \tag{2.35}$$

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

$$P = NR/\beta kA, \tag{2.36}$$

where we have taken A to the other side of the equation.[6] 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, (2.36)

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

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

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).

The final step in this exploration of a deepening analogy is to link the thermodynamics with the statistical mechanics that generated the flow models. In physics, this is achieved by connecting the free energy to the partition function of the system of interest. We saw in the transport case that while we could find analogues of partition functions, the analogy was not exact.[7]

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

$$Z_i = \Sigma_k \exp(\alpha \log W_k - \beta c_{ik}). \tag{2.37}$$

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:

$$Z = \Sigma_i Z_i = \Sigma_{ik} \exp(\alpha \log W_k - \beta c_{ik}). \tag{2.38}$$

We can then seek to work with the free energy and the model at (2.16) and (2.26). Then, using (2.8):

$$F = -[N/\beta] \log Z. \tag{2.39}$$

We can also explore the standard method of calculating state functions from the free energy:[9]

$$P = -(\partial F/\partial A)_T, \tag{2.40}$$

$$S = -(\partial F/\partial T)_A, \tag{2.41}$$

or, using (2.16):

$$S = -k\beta^2(\partial F/\partial \beta)_A. \tag{2.42}$$

[7] 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 (2.11) specifies the energy and β (=$1/kT$) the temperature, then $F = U - TS$ becomes $F = C - S/k\beta$? Then if $F = NkT \log Z$, what is Z?

[8] ter Haar (1995, 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] The following equations can be derived from (2.31) with A substituted for V and $T = 1/k\beta$.

And, with $U=C$, using (2.23),

$$U = F - (\partial F/\partial T)_A = -T^2(\partial/\partial T \cdot F/T)_A = (\partial/\partial\beta \cdot k\beta F)_A. \qquad (2.43)^{10}$$

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 (2.40) as:

$$X_i = -(\partial F/\partial x_i)_T. \qquad (2.44)$$

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 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. The standard formulae for specific heats can be transformed into the urban formalism as follows:

$$C_V = (\partial U/\partial T)_V \to -1/k\beta^2(\partial U/\partial\beta)_A, \qquad (2.45)$$

and

$$C_P = (\partial U/\partial T)_P + P(\partial V/\partial T)_P = [-1/k\beta^2(\partial U/\partial\beta)_P + P(\partial V/\partial\beta)_P]. \qquad (2.46)$$

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.[11]

It remains to ask the question of whether there could be phase changes in spatial interaction systems.[12] 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.

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[10] What does this produce for U? And is it possible to do all the calculations implied by (2.40)–(2.46)?

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

[12] We elaborate the notion of phase changes in the next section. Essentially, in this case, they would be discrete "jumps" in the $\{T_{ij}\}$ or $\{S_{ij}\}$ arrays at critical values of parameters such as β.

2.3 Urban Structure and its Evolution

2.3.1 The Model

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):

$$dW_j/dt = \varepsilon(D_j - KW_j)W_j, \tag{2.47}$$

where K is a constant such that KW_j can be taken as the (notional) cost of running the shopping centre in j.[13] This equation then says that if the centre at j is profitable, it grows; if not, it declines. The parameter ε determines the speed of response to these signals.

The equilibrium position is given by:

$$D_j = KW_j, \tag{2.48}$$

which can be written out in full, using (2.23), as:

$$\Sigma i\{e_i P_i W_j \exp(-\beta c_{ij})/\Sigma_k W_k \exp(-\beta c_{ik})\} = KW_j. \tag{2.49}$$

The (2.47) 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 2008).

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.[14] This can be interpreted to an extent for a particular zone, say j, by fixing all the W_k, for $k \neq j$. A key challenge is to solve this problem with all the W_js varying simultaneously. There are many procedures for solving (2.49) iteratively but we constantly need to bear in mind the sensitivity to the initial conditions.

The zonal interpretation is shown in Fig. 2.1. The left and right hand sides of (2.49) 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 ($\alpha = 1$) case that joins the two. The β value also

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

[14] Clarke and Wilson (1985).

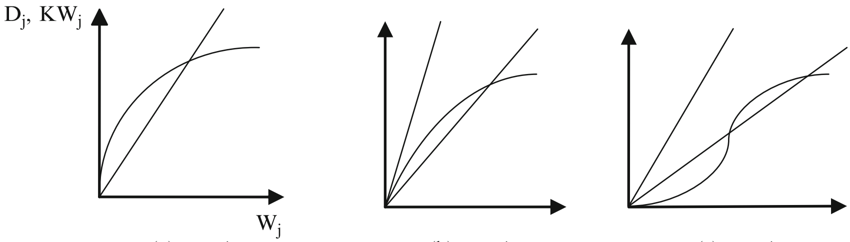

Fig. 2.1 Zonal analysis of phase transitions

determines the 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 Fig. 2.1b, c]. These kinds of change can be characterised as phase transitions – in this case at a zonal level, but clearly there will be system wide changes of this kind as well. This analysis is the basis of a very powerful tool for identifying complex phase transitions. We return to this in the Sect. 2.4.6.

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, recognizing the points at which phase changes take place. This is where newer statistical mechanics models potentially can help.

This analysis exemplifies characteristics of models of nonlinear complex systems: multiple equilibrium solutions, path dependence and phase transitions and so demonstrate the contribution of urban modelling to complexity science.

2.3.2 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. This differs from a microcanonical ensemble in that the energy is allowed to vary. The return to equilibrium after a disturbance 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 Physics, 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 nested in the canonical distribution for each energy value in the latter.

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:

$$P_r = \exp(-\beta H_r)/\Sigma_r \exp(-\beta H_r). \tag{2.50}$$

Physicists have modelled the distribution of states of particles on a lattice. An early example was the Ising model which is concerned with spin systems and the alignment of spins at certain temperatures that produce magnetic fields. 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 – see Martin (1991).

Locations in urban systems can be characterised by grids and urban structure can then be thought of as structure at points on a lattice. 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 (2.50) as:

$$P_r = \exp(-\beta H_r(\{W_j\}))/\Sigma_r \exp(-\beta H_r(\{W_j\})), \tag{2.51}$$

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

$$L\left[\{W_j^{\text{opt}}\}\right] = \text{Max}_r \exp(-\beta H_r(\{W_j\})). \tag{2.52}$$

So the immediate issue is to decide on the Hamiltonian. Suppose we take the measure of profit used in (2.47). Then:

$$H = \Sigma_j(D_j - KW_j), \tag{2.53}$$

and the problem becomes:

$$L\left[\{W_j^{\text{opt}}\}\right] = \text{Max}_r \exp[-\beta\Sigma_j(D_j - KW_j)], \tag{2.54}$$

where K is a unit cost for retailers and D_j can be obtained in the usual way. Substitution then gives:

$$L\left[\{W_j^{\text{opt}}\}\right] = \text{Max}_r \exp[-\beta\Sigma_j(\Sigma_i\{e_iP_iW_j \exp(-\beta c_{ij})/\Sigma_k W_k \exp(-\beta c_{ik})\}KW_j)], \tag{2.55}$$

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

$$\Sigma_j(\Sigma_i\{e_iP_iW_j \exp(-\beta c_{ij})/\Sigma_k W_k \exp(-\beta c_{ik})\} - KW_j), \tag{2.56}$$

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:

$$\Sigma_i\{e_iP_iW_j \exp(-\beta c_{ij})/\Sigma_k W_k \exp(-\beta c_{ik})\} = KW_j, \tag{2.57}$$

which is, of course, simply the equilibrium condition (2.48) [or (2.49)]. 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 Fig. 2.1 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.[15] There is also the interesting possibility that entropy is used as a measure of dispersion and so $-\Sigma_j W_j \log W_j$ could be used as an order parameter.[16]

2.3.3 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. It is interesting to explore the possibility of a suboptimal $\{W_j\}$ via entropy maximizing – 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 them from the transportation problem of linear programming (and, of course, as we noted earlier, it has been shown that as $\beta \to \infty$, the spatial interaction model solution tends to the linear programming limit). We can proceed as follows. Assume $\{S_{ij}\}$ is given.[17] Then maximise an entropy function in $\{W_j\}$ subject to appropriate constraints.

$$\text{Max } S = -\Sigma_j W_j \log W_j, \tag{2.58}$$

such that

$$\Sigma_{ij} S_{ij} \log W_j = X, \tag{2.59}$$

[15] 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?

[16] I am grateful to Aura Reggiani for this suggestion.

[17] It can be shown that we can carry out an entropy maximizing calculation on $\{S_{ij}\}$ simultaneously and that leads to a conventional a spatial interaction 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 spatial interaction model and then iterate with $\{W_j\}$.

and

$$\Sigma_i S_{ij} = kW_j + Y, \tag{2.60}$$

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 (2.48) is being treated as suboptimal. The Lagrangian for this problem is:

$$L = -\Sigma_j W_j \log W_j - \mu\Sigma_i[S_{ij} - KW_j - Y] - \alpha(\Sigma_i S_{ij})/W_j, \tag{2.61}$$

and setting

$$\partial L/\partial W_j = 0 \tag{2.62}$$

gives, with some re-arrangement,

$$\log W_j + \alpha D_j/W_j = \mu K_j \tag{2.63}$$

(where we have substituted D_j for $\Sigma_i S_{ij}$ without loss of generality since we are taking the $\{S_{ij}\}$ as fixed). These equations could be solved numerically for $\{W_j\}$ – and indeed graphically.

It is then interesting to interpret (2.63) and then to look at the $\alpha \to \infty$ limit. Write (2.63), by dividing by μ, as follows:

$$(1/\mu)\log W_j + \alpha D_j/\mu W_j = K_j. \tag{2.64}$$

The left 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 (2.64) 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 (2.64) then clearly tends to 0 and the equation then becomes equivalent to (2.48).

2.4 Ongoing Challenges

2.4.1 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?

2.4.2 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 chapter but it would be useful, for example, to expound more fully the external variables that underpin changes in these systems.

2.4.3 Development and Evolution

The structural evolution 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 (that is, cost) functions to see whether new kinds of phase transitions would emerge. 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! Finally, huge progress has been made in the development of comprehensive models and these also should be explored for phase transitions.

2.4.4 The "New" Thermodynamics and Statistical Mechanics

We noted at the outset that authors such as Ruelle (2004) and Beck and Schlagel (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 chapter into these formats to explore the extent to which further advances are possible. We have only scratched the surface of possibilities in this chapter and further research is to be encouraged.

2.4.5 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 on 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 (et al.'s) work on free energy and the brain. It is interesting to place this model into a planning framework. 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.

2.4.6 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 generalizing 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 taking 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 $\{W_j\}$ 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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