An introduction to phase transitions in stochastic dynamical systems

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Abstract. We give an introduction to phase transitions in the steady states of systems that evolve stochastically with equilibrium and nonequilibrium dynamics, the latter defined as those that do not possess a time-reversal symmetry. We try as much as possible to discuss both cases within the same conceptual framework, focussing on dynamically attractive ‘peaks’ in state space. A quantitative characterisation of these peaks leads to expressions for the partition function and free energy that extend from equilibrium steady states to their nonequilibrium counterparts. We show that for certain classes of nonequilibrium systems that have been exactly solved, these expressions provide precise predictions of their macroscopic phase behaviour.

1. Introduction
It is highly desirable that we properly understand the role of microscopic dynamics in shaping the macroscopic properties of many-body interacting systems. This was highlighted many times during the recent Summer School on “Ageing and the Glass Transition” [1] where the microscopic origins of glassy behaviour were much debated [2, 3]. Macroscopically, one sees at the glass transition diverging relaxational timescales—manifestly dynamical quantities—e.g., the viscosity of a fluid increasing by many orders or magnitude [4, 5]. One prominent macroscopic effect in the glassy phase is ageing [6], where experimental observables depend on the overall time since the glass was formed. A microscopic picture often used to explain such behaviour has particles being caged by their nearest neighbours, thus impeding relaxation to equilibrium. Meanwhile, spin glass systems [7, 8] exhibit exotic memory and rejuvenation effects in their glassy phase. Here, a microscopic dynamical explanation involves the exploration of complex free-energy landscapes with many nested minima. More generally there is a drive to understand complexity in all manner of dynamically interacting systems, such as societies, ecosystems, geological structures and so on (see, e.g., [9] for an introduction).

If one is dealing with a system that is not subject to a driving force, equilibrium statistical mechanics provides a complete theory for deriving macroscopic properties from a microscopic model. This success perhaps gives us hope that we may be able to extend such theories to nonequilibrium systems, e.g., the glassy and complex systems described above and which are typically couched in terms of microscopic dynamical rules. A problem here is that the equilibrium theory makes little reference to the latter, other than the tendency for equilibrium dynamics to maximise disorder. To understand the consequences of enforcing nonequilibrium dynamics—specifically those that drive the system away from thermal equilibrium—I focus exclusively on the macroscopic phenomenon of the phase transition. In order to make connections between...
phase transitions in equilibrium and nonequilibrium steady states, I shall revisit the former
from the viewpoint of a dynamical phase-space exploration. It is therefore necessary to be clear
about the distinction between equilibrium and nonequilibrium dynamics. This is where I begin.

2. Equilibrium and nonequilibrium stochastic dynamics
Consider a system of classical particles in thermal equilibrium with a heat bath at inverse
temperature $\beta = 1/kT$. Although the trajectories of these particles can in principle be predicted
from Newton’s deterministic equations of motion, it is appropriate to use a stochastic description
of the dynamics due to the complexity in the dynamics resulting from the vast number of
collisions that take place (see, e.g., [10, 11]). A further indeterminacy lies in fact that the
precise nature of the interaction between the system and the heat bath is often unspecified.

We express these stochastic rules using the probabilities $M_{\delta t}(C \rightarrow C', t)$ that the system
evolves from a configuration (point in phase-space) $C$ at time $t$ to reach a new configuration $C'$
after a time interval $\delta t$. Note that one can employ a discrete-time stochastic model even when
the underlying dynamics are continuous. We now identify four properties this stochastic process
should possess in order to model the evolution of a system at equilibrium.

(i) **Markov property** — The transition probabilities $M_{\delta t}(C \rightarrow C', t)$ are assumed not to depend
on the history of the process prior to time $t$. This is appropriate because, given the phase-
space coordinates $C$ at time $t$ one could, in principle, calculate the transition probabilities
without this historical information.

(ii) **Time translational invariance** — When a system is not being driven by an external force,
the underlying equations of motion are time-translationally invariant, and so we can drop
the dependence of the transition probabilities on time.

(iii) **Ergodicity** — An important property of many-body dynamical systems is that of ergodicity,
in which a quantity averaged over a single trajectory equals that taken over the stationary
distribution of configurations obtained from many different initial conditions [11]. In the
context of stochastic processes in a finite state space, ergodicity is the property of there
being a unique stationary distribution that is converged on from every initial condition and
for every configuration to be represented by a nonzero probability in this distribution$^1$.

(iv) **Time reversal symmetry** — At equilibrium, the ensemble of realisations of the dynamics
running forwards in time cannot be distinguished from that of those running backwards.

This is because the underlying equations of motion have this property [10]. Furthermore,
there is no “arrow of time” once the maximum-entropy equilibrium state has been reached.

There is only enough space here to highlight the most important consequences of these properties;
for full details, the reader should consult textbooks on stochastic processes, such as [10, 12].

Together, properties (i) and (ii) imply that we can describe the evolution of the probability
distribution over state-space $P(C)$ in terms of a master equation

$$P(C, t + \delta t) = \sum_{C'} P(C', t)M_{\delta t}(C' \rightarrow C) .$$  \hspace{1cm} (1)

In order for a stochastic process to be ergodic [property (iii)], the dynamics must allow every
configuration $C'$ to be reached from any other configuration $C$ after a fixed (but possibly large)
number of transitions. Whether ergodic or not, probability must be conserved by the dynamics:
$\sum_{C'} M_{\delta t}(C \rightarrow C') = 1$. Then, we can write (1) as

$$P(C, t + \delta t) - P(C, t) = \sum_{C' \neq C} [P(C', t)M_{\delta t}(C' \rightarrow C) - P(C, t)M_{\delta t}(C \rightarrow C')] . \hspace{1cm} (2)$$

$^1$ Actually, one can find in the literature a number of different definitions of ergodicity. The one given here is the
most restrictive and agrees with that found in, say, [12].
The first term on the right-hand side of this equation gives the gain in probability from transitions into the state $\mathcal{C}$, and the second term the loss from transitions out of $\mathcal{C}$. A steady state is reached when $P(\mathcal{C}, t + \delta t) = P(\mathcal{C}, t) \equiv P^*(\mathcal{C})$ and the total loss and gain terms balance. The very special case where the losses and gains cancel term-by-term in (2) is called detailed balance \cite{10, 12}, i.e.,

$$P^*(\mathcal{C}) M(\mathcal{C} \to \mathcal{C}') = P^*(\mathcal{C}') M(\mathcal{C}' \to \mathcal{C}).$$

(3)

This particular balancing of the loss and gain is required to satisfy the time-reversal symmetry property (iv). This one sees from the fact that (iv) implies that in the steady state, the probability of observing a particular trajectory $\mathcal{C}_0 \to \mathcal{C}_1 \to \mathcal{C}_2 \cdots \to \mathcal{C}_N$ equals that of its time reversal. That is, we must have

$$P^*(\mathcal{C}_0) M_{\delta t}(\mathcal{C}_0 \to \mathcal{C}_1) M_{\delta t}(\mathcal{C}_1 \to \mathcal{C}_2) \cdots M_{\delta t}(\mathcal{C}_{N-1} \to \mathcal{C}_N) = P^*(\mathcal{C}_N) M_{\delta t}(\mathcal{C}_N \to \mathcal{C}_{N-1}) M_{\delta t}(\mathcal{C}_{N-1} \to \mathcal{C}_{N-2}) \cdots M_{\delta t}(\mathcal{C}_1 \to \mathcal{C}_0)$$

(4)

for all trajectories of any length $N$ \cite{12}. The special case $N = 1$ reduces to the detailed balance condition (3). Note also that if one forms a loop in state space by putting $\mathcal{C}_N = \mathcal{C}_0$ one obtains the Kolmogorov criterion \cite{12}

$$M_{\delta t}(\mathcal{C}_0 \to \mathcal{C}_1) M_{\delta t}(\mathcal{C}_1 \to \mathcal{C}_2) \cdots M_{\delta t}(\mathcal{C}_{N-1} \to \mathcal{C}_N) = M_{\delta t}(\mathcal{C}_N \to \mathcal{C}_{N-1}) M_{\delta t}(\mathcal{C}_{N-1} \to \mathcal{C}_{N-2}) \cdots M_{\delta t}(\mathcal{C}_1 \to \mathcal{C}_0)$$

(5)

which is an equivalent statement of detailed balance. This expression is useful because often when formulating a stochastic dynamical model (e.g., to describe nonequilibrium or complex systems as described in the Introduction) one does not know the stationary distribution $P^*(\mathcal{C})$ in advance, only the transition probabilities $M_{\delta t}(\mathcal{C} \to \mathcal{C}')$. Since (5) contains only the latter, one can establish whether or not the steady state is time-reversal symmetric or not. If it is, one can then find a potential function $V(\mathcal{C})$ that is uniquely defined in terms of the differences

$$V(\mathcal{C}') - V(\mathcal{C}) = \frac{1}{\beta} \ln \left[ \frac{M_{\delta t}(\mathcal{C}' \to \mathcal{C})}{M_{\delta t}(\mathcal{C} \to \mathcal{C}')} \right]$$

(6)

for pairs of configurations between which transitions in a single timestep occur. In other words, summing these differences along any path between two configurations always gives the same result, implying that forces are conservative and that the stationary distribution is Boltzmann: $P^*(\mathcal{C}) \propto \exp[-\beta V(\mathcal{C})]$.

Conversely, in the absence of time reversal symmetry, a potential function defined via (6) becomes multivalued: forces are then nonconservative and the dynamics dissipate energy. Furthermore, (5) implies a circulation of probability in the steady state, which are likely to be manifested as macroscopic currents. These decidedly nonequilibrium effects lead us to conclude that the defining property of nonequilibrium dynamics is a lack time-reversal symmetry in the steady state: i.e., dynamics for which none of the (equivalent) conditions (3), (4) and (5) hold.

3. Phase transitions from a microscopic dynamical point of view

We now describe how a stochastic dynamics—assumed Markov, time-translationally invariant and ergodic, but not necessarily time-reversal symmetric—is drawn to particular regions of configuration space. Such considerations are paramount in Monte Carlo simulation and so descriptions similar to the following can be found in textbooks on the subject such as \cite{13}.

For concreteness, we base our discussion around a hypothetical, doubly-peaked steady-state distribution $h(\epsilon)$ of a macroscopic quantity $\epsilon$ which we notionally take to be an energy density—see Fig. 1. We shall associate the lower-energy peak with an ordered (solid) phase, and the
Figure 1. Exploration of a doubly-peaked stationary distribution whose weight shifts between peaks as the inverse temperature $\beta$ is decreased.

higher-energy peak with a disordered (fluid) phase. One can define the weight (area) of the distribution under a peak as being proportional to the time a dynamical trajectory—whether equilibrium or nonequilibrium—spends under that peak, as the length of that trajectory tends to infinity. Equivalently (because the process is ergodic [12]), this distribution is given by the stationary solution of the master equation (1). Either way, a phase transition occurs—roughly speaking—at a critical value of an external parameter $\beta$ (notionally, inverse temperature) at which peak containing the majority weight changes, as shown in Fig. 1.

To be more precise, let us assume that for sufficiently large volumes $V$, the statistical weight (unnormalised probability) $h(\epsilon)$ of the macrostate $\epsilon$ can be expressed in the from

$$h(\epsilon) \approx e^{-\beta V g_{\beta}(\epsilon)}$$

in which the function $g_{\beta}(\epsilon)$ is independent of $V$ but changes with $\beta$. We base this assumption on the fact that at equilibrium, $g_{\beta}(\epsilon)$ is a free-energy density—there is, however, no reason to assume that this statement is generally true. Nevertheless, we shall persevere with this assumption in order to investigate the thermodynamic (infinite volume) limit.

Consider first the situation shown in Fig. 1 where the two phases corresponding to the peaks are not related by a symmetry transformation (as is the case for a fluid and a solid). Approximating each peak by a Gaussian, it is easy to show that the ratio of weights under the peaks grows exponentially with volume as $\exp(-\beta V [g_{\beta}(\epsilon_1) - g_{\beta}(\epsilon_2)])$. Thus the peak with the greater height—or lowest free energy $g(\epsilon)$—is overwhelmingly dominant in the thermodynamic limit. Furthermore, this overwhelming dominance shifts suddenly from one region of state space to another at the temperature at which one peak height overtakes the other. It is this sudden change, described mathematically by a sharp discontinuity in the limit of infinite volume, that is the defining property of a phase transition.

At the transition point where both peaks have the same height, each possesses a non-vanishing fraction of the total weight. This corresponds to the physical phenomenon of phase coexistence which, along with latent heat, is a signature of an equilibrium first-order transition. Near the transition, where the difference in peak heights is not too great, an initial condition under the smaller peak can persist for long times indicating the presence of metastability which is also typically observed near a first-order equilibrium phase transition. Although the lifetime of the metastable phase depends on the distance from the transition point and the precise nature of the stochastic dynamical rules (whether time-reversal symmetric or not), one expects by analogy with a Kramers problem for the escape of a potential well through diffusion [14, 15] that it will grow exponentially in the system’s volume.

A different situation occurs at a transition at which a single peak splits into two (or more) symmetric peaks as shown in Fig. 2. This occurs, for example, if a paramagnet spontaneously orders as the temperature is lowered. The symmetry implies that for a whole range of temperatures (not just at a single point), each peak has precisely the same area. Although,
given long enough, an ergodic dynamics would then spend the same amount of time in each phase, it turns out again that the time taken to surmount the barrier between the phases grows exponentially with the volume and so in the thermodynamic limit, the dynamics only get to explore the peak under which they start. This describes a symmetry-breaking transition.

At equilibrium such continuous transitions are typically accompanied by diverging correlation lengths and times.

In this description of phase transitions we have assumed only a general property of peaks in the stationary distribution and ergodic—but not necessarily equilibrium—dynamics. However, it is worth for a moment specialising to the equilibrium case where much more is known. As noted above, the function $g(\epsilon)$ is then a free energy that the dynamics tend to minimise. Macroscopically, one can often ascribe a phase transition to a competition between minimising the energy and maximising the entropy, the relative balance of the two controlled by the temperature. It is interesting to observe that this competition is also a feature of a stochastic equilibrium dynamics.

Let us consider as a concrete example the Metropolis algorithm which is popular in Monte Carlo simulation as a method to generate a sequence of configurations that samples an equilibrium distribution [16, 17]. It is implemented by repeatedly iterating two steps:

(i) Given a configuration $C$, one generates a trial subsequent configuration $C'$ using a stochastic rule that, on its own, is time-reversal symmetric with respect to a uniform distribution over state space. For example, in an Ising model, one could flip a randomly-chosen spin.

(ii) If $C'$ has a lower energy than $C$, it is always used as the next configuration in the sequence. Otherwise, it is retained only with a probability $e^{-\beta[E(C') - E(C)]}$.

From the discussion of the previous section, it is straightforward to show that these dynamics generate time-reversal symmetric trajectories sampling the Boltzmann distribution $P^*(C) \propto e^{-\beta E(C)}$. Notice particularly how the energy-entropy competition arises: step (i) generates an attraction towards high-entropy macrostates (i.e., those that are realised by a large number of microstates) whilst step (ii) repels those high-entropy states that involve too great an increase in energy.

4. Mathematical characterisation of discontinuities at a phase transition

In the previous section we found that under the assumption of the statistical weight of macrostates varying with system volume $V$ according to (7), an overwhelmingly large proportion of the weight resides under the peak with the greater height in the limit of infinite $V$. Therefore, the normalisation of this weight function

$$Z(\beta) = \int d\epsilon h(\epsilon) \approx \int d\epsilon e^{-\beta V g_\beta(\epsilon)}$$

(8)
closely approximates the area under the highest peak (or peaks when more than one have the same height). Approximating once again the peaks as Gaussians one finds that

$$f(\beta) = -\lim_{V \to \infty} \frac{\ln Z(\beta)}{\beta V} = \min_{\epsilon} \{g_\beta(\epsilon)\}$$

(9)
gives the free-energy-like quantity corresponding to the highest peak(s). At equilibrium, \( f(\beta) \) is the equilibrium (Helmholtz) free energy density and, as is well understood (see e.g., [18]) signals a phase transition through a nonanalyticity in \( f(\beta) \). In particular, a discontinuous first derivative implies a jump in a quantity like the energy or density of the system, i.e., a first-order transition, whilst a discontinuous higher derivative corresponds to a continuous transition.

Under the assumption that the peaks of a stationary distribution arising from nonequilibrium dynamics behave according to (7), we can always characterise the height of the largest peak using the normalisation of the distribution \( Z(\beta) \) in exactly the same way as we do for an equilibrium distribution to find the equilibrium free energy. What is missing is a general expression for the normalisation and any association between particular nonanalyticities in the resulting free energy (9) and macroscopically observable behaviour. In the remainder of this article we address these points.

First, we show that it is possible to write down a general expression for the normalisation \( Z(\beta) \) (see also [19]). This is achieved by casting the master equation (2) as a matrix equation

\[
P(t + \delta t) - P(t) = MP(t)
\]

in which the \( i \)th element of \( P(t) \) gives the probability for the system to be in configuration \( C_i \) at time \( t \), the off-diagonal matrix elements \( |M|_{ij} = M_{ij}(C_j \rightarrow C_i) \) encode the gain terms and the diagonal matrix elements the loss terms \( |M|_{ii} = - \sum_j M_{ij}(C_i \rightarrow C_j) \). After imposing a normalisation constraint, Cramer’s rule [20] can be employed to solve the matrix equation \( MP^* = 0 \) for the stationary distribution \( P^* \). This procedure gives

\[
P^*(C_i) = \frac{\det \tilde{M}^{(i)}}{Z} \quad \text{with} \quad Z = \sum_i \det \tilde{M}^{(i)}.
\]

where \( \tilde{M}^{(i)} \) is the matrix obtained by striking out both row and column \( i \) of \( M \). We shall use the normalisation \( Z \) that arises through this procedure to define a generalised partition function for any system with a unique steady state, whether equilibrium or nonequilibrium.

This form of \( Z \) implies, via the matrix tree theorem [21, 22, 23], that it is the partition function for an ensemble of spanning in-trees on the graph of transition probabilities with a particular edge weighted by its corresponding transition probability \( M(C \rightarrow C') \). This suggests an interpretation (albeit abstract) of the transition probabilities as equilibrium fugacities: we shall see this more concretely later. In the meantime, we note that a drawback of (11) is that calculation of the determinants is intractable for a model with even a modest number of microstates, let alone in the thermodynamic limit of infinite volume which is required for a free energy to develop a nonanalyticity, and thereby predict a phase transition.

One way to gauge the possibility of a phase transition in an infinite system when one only has finite-size results to hand is to look at the zeros of the partition function in the complex plane of external parameters (in this context, the transition rates), an approach that was introduced by Lee and Yang in the 1950s [24, 25]. The historical development of these ideas, and their application to both equilibrium and nonequilibrium steady states, has recently been very thoroughly reviewed in [26], an effort that extends our own overview of the nonequilibrium cases in [27]. Therefore, we cover only the most salient points here.

For simplicity, let us assume that every nonzero transition probability is some integer power of an external parameter \( z \) (e.g., in an Ising model one might have \( z = e^{-\beta} \)). Eq. (11) then implies that the partition function \( Z \) is a polynomial in \( z \), its zeros lying off the positive real axis in the complex-\( z \) plane because \( Z \) is a sum of positive statistical weights. This means that the free energy, obtained from the partition function using (9), has only isolated logarithmic singularities in the complex plane, and hence is analytic for the entire range of \( z \) that can be accessed physically (i.e., the positive real \( z \) axis).
The only exception to this is if zeros approach a point $z_c$ on the positive real axis arbitrarily closely in the thermodynamic limit. It turns out that typically the zeros approach $z_c$ along a line $\text{Re} f_1(z) = \text{Re} f_2(z)$ separating two different analytic free energies $f_1(z)$ and $f_2(z)$. By expanding the free energy difference between the two phases near the transition point $z_c$, one finds (see [26, 27] for details and original references) that if the free energy has a discontinuity in its first derivative, as it would at an equilibrium first-order transition, the line of zeros passes smoothly along a parabola through $z_c$ and with a non-vanishing density of zeros at that point. At a point where a higher derivative is discontinuous (as occurs at an equilibrium continuous transition) the density of zeros vanishes as the critical point is approached, the path forming a cusp. These characteristics are indicated schematically in Fig. 3. Thus we see that the zeros of the partition function give a nice way to represent nonanalyticities in the associated free energy which, in turn, relate to structural changes in peaks of the stationary distribution as described in Section 3. Recall, however, that we have no general theory to suggest that, for example, a discontinuity in the first derivative of the free energy necessarily implies that the physical phenomena associated with a first-order transition will be observed in a nonequilibrium steady state. This possibility we now explore with reference to an exactly solved model.

### 5. Case study: The asymmetric exclusion process with open boundaries

The asymmetric exclusion process (ASEP) with open boundaries is an exemplar of an interacting particle system that is driven by its environment. Introduced as a model of biopolymerisation [28], and relevant also to the study of traffic flow [29] and biological transport [30], it comprises a one-dimensional lattice of $L$ sites, each of which may be occupied by at most one particle by virtue of a hard-core exclusion constraint. In a timestep of duration $\delta t$, a particle in the bulk hops one site to the right with probability $\alpha\delta t$ as long as the hard-core exclusion constraint is not violated as a result. Additionally, the left-most site can—if empty—be populated with a particle with probability $\alpha\delta t$ and a particle at the rightmost site removed with probability $\beta\delta t$. These transitions are illustrated in Fig. 4. We consider the continuous-time limit $\delta t \to 0$ so that at most one event occurs in a timestep: this defines a random-sequential updating scheme in which $\alpha$ and $\beta$ are transition rates. The fact that no elementary particle move can immediately be reversed implies a lack of time-reversal symmetry in the dynamics. Particularly, there is a nonzero particle current in its nonequilibrium steady state.

The main reason for discussing the model in the present work is that its steady-state
distribution has been calculated exactly through two different (but equivalent) approaches [31, 32]. In particular this means such properties as the partition function, free energy, peaks in the distribution and so on can be extracted and compared with the macroscopic phase behaviour present in the model. There are, in fact, three distinct phases in the steady state:

(i) **High-density (HD) phase** — When the exit rate $\beta$ is lower than the entry rate $\alpha$ and further smaller than a critical value of $\frac{1}{2}$, particles accumulate at the right boundary creating a region of high density $\rho = 1 - \beta$ that extends into the bulk, before decaying exponentially towards the left boundary. The slow exit rate further limits the current to $J = \beta(1 - \beta)$.

(ii) **Low-density (LD) phase** — Since the system is invariant under the combined transformation of a particle-hole exchange and left-right reflection of the lattice, it follows that for $\alpha < \beta, \alpha < \frac{1}{2}$ one has a transformed version of the HD phase. This has a low density $\rho = \alpha$ extending from the left boundary into the bulk along with an exponential decay from the right boundary and a current $J = \alpha(1 - \alpha)$.

(iii) **Maximal-current (MC) phase** — When both entry and exit rates $\alpha$ and $\beta$ are greater than $\frac{1}{2}$, the boundaries no longer limit the current and instead a particle’s progress is impeded by the hard-core exclusion. In this phase the current assumes a constant value $J = \frac{1}{4}$, the maximum for any combination of $\alpha$ and $\beta$. The density is $\rho = \frac{1}{2}$ in the bulk and has a power-law decay with exponent $\frac{1}{2}$ both from the left and towards the right boundary.

The phase diagram is shown in Fig. 5 (i).

We are particularly interested in the physics near the transition points. Along the boundary between the HD and LD phases, $\alpha = \beta < \frac{1}{2}$, there is phase coexistence with low- and high-density regions separated by a shock front that performs a random walk along the lattice [33]. This phenomenology, shown in Fig. 5 (ii), is reminiscent of an equilibrium first-order transition. Meanwhile as the MC phase is approached from either the LD or HD phase, the lengthscale characterising the density decay diverges, as often occurs at a continuous equilibrium phase transition but with power-law correlations exhibited generically in the MC phase. See Fig. 5 (iii).

The partition function (11) for an $L$-site lattice is known from the exact solutions [31, 32] to be

$$Z_L = \sum_{n=0}^{L} \frac{(L-n)(L+n-1)!}{L!n!} (\alpha\beta)^n \sum_{r=0}^{L-n} \alpha^r \beta^{L-n-r}. \quad (12)$$

Note that the expression in [32] omits an unimportant factor of $(\alpha\beta)^L$ which is present if one follows through the solution employing matrix determinants (11).
Figure 6. Zeros of the ASEP’s partition function (12) for a lattice of \( L = 300 \) sites in the complex-\( \alpha \) plane. For \( \beta = \frac{1}{3} \), a first-order phase transition occurs at \( \alpha = \frac{1}{3} \). At \( \beta = 1 \) a continuous transition at \( \alpha = \frac{1}{2} \) occurs. The dashed line shows the phase-boundary determined analytically [34] for the latter case.

Figure 7. An equilibrium surface whose partition function coincides with that for the ASEP. The arrows indicate contacts with the origin which lower the surface’s energy whilst entropy is gained from excursions away from the origin, such as that shown shaded.

We explore the nonanalyticities in the free energy (9) by examining the zeros of this partition function for a finite system, as described in the previous section. Here, we go into the complex-\( \alpha \) plane at fixed \( \beta \) (without loss of generality, because of the symmetry under the exchange \( \alpha \leftrightarrow \beta \) and of particles and holes). In Fig. 6, numerical solutions for the zeros with \( \beta = \frac{1}{3} \) and \( \beta = 1 \), both with \( L = 300 \) are shown. In the former case the path of zeros passes smoothly through a point on the real axis with \( \alpha \approx \frac{1}{3} \). Meanwhile, in the latter case we have a path of zeros meeting at an angle of \( \pi/2 \). As previously described, these patterns are characteristic of equilibrium first-order and continuous phase transitions and the physical phenomena seen at the transitions (see above) correspond with these classifications. This result is quite intriguing given that the logarithm of (12) is not an equilibrium free energy, nor are \( \alpha \) and \( \beta \) equilibrium fugacities. One can attempt to explain this result by noting that the free energy and current are simply related [32] via \( f(\alpha, \beta) = \ln J(\alpha, \beta) - \ln \alpha \beta \), a fact that allows the locus of partition function zeros to be determined analytically [34]. However, this explanation amounts to a statement that the correct order parameters to characterise the phase transitions are the derivatives of \( J \) with respect to \( \alpha \) and \( \beta \)—a statement which I do not find obvious.

To turn full circle, I conclude by examining peaks in the ASEP’s stationary distribution. It is possible, though technically difficult, to determine the distribution over the time-integrated current [35], instantaneous current-density [36] and even spatially-dependent density profile [37] microstates. Here, we take a short-cut which brings additional insight in terms of an energy-entropy competition at the expense of losing sight of the dynamics.

The idea is to construct an \textit{equilibrium} statistical mechanical model whose partition function coincides with (12). One prescription [23, 38] is a surface on a one-dimensional surface whose left
Figure 8. Peaks in the $\rho_a$-$\rho_b$ plane (labelled $x$ and $y$ respectively in the figures) for a large, but finite, surface length $L$. From left to right: $\alpha = \frac{3}{4}, \beta = \frac{7}{10}; \alpha = \frac{7}{8}, \beta = \frac{2}{3};$ and $\alpha = \beta = \frac{1}{3}$.

portion is constrained to lie above an origin and its right portion below—see Fig. 7. Contacts with the origin from above (respectively, below) contribute an energy $\ln \alpha$ ($\ln \beta$). Note that $\alpha$ and $\beta$ are equilibrium fugacities in this interpretation, and when sufficiently small allow the lowering of the energy by contact with the origin to beat the entropy gained from large excursions of the surface from the origin. This competition gives rise to three equilibrium phases: one in which the surface is adsorbed from above, one from below and a third in which it is completely desorbed. These correspond to the ASEP's LD, HD and MC phases respectively, and the phase diagram is exactly the same as in Fig. 5 (i) (as it must be). Furthermore, the preceding classification of the transitions is uncontroversial in this picture since derivatives of the free energy with respect to $\alpha$ and $\beta$ give the appropriate order parameters for the model, viz, the density $\rho_a$ of contacts with the origin from above and $\rho_b$ from below.

In the space spanned by these order parameters, the stationary distribution is [23, 39]

$$h(\rho_a, \rho_b) \sim \left[ \frac{(2 - \rho_a - \rho_b)^{2-\rho_a-\rho_b}}{\alpha^{\rho_a} \beta^{\rho_b}(1 - \rho_a - \rho_b)^{1-\rho_a-\rho_b}} \right]^L$$

which has the exponential growth with system size $L$ prescribed in Section 3. As can be seen from Fig. 8, the three equilibrium phases correspond to peaks on the boundary of the physical region $0 \leq \rho_a + \rho_b \leq 1$. In the HD phase (adsorption from above), the dominant peak is at a point with $\rho_a = 0, \rho_b > 0$, whilst the peak corresponding to the LD phase (adsorption from below) on the line $\rho_b = 0$ in exponentially suppressed. In the entropy-dominated desorbed phase, these two peaks merge into one at $\rho_a = \rho_b = 0$. This is reminiscent of the discussion of the continuous phase transition in Section 3, although in the present case no symmetry breaking is involved. At the first-order transition, the situation is a little different to that described in Section 3. Rather than two isolated peaks of equal height, we have a continuous ridge linking the LD and HD phase peaks. That is, any mixture of these two phases is represented with equal weight in this distribution, a fact that is reflected in the diffusive wandering of the shock front separating them in the ASEP (discussed above): indeed, one also finds this feature in the distribution in the density-current plane [36]. Thus we see that, broadly speaking at least, the general features outlined in Section 3 are present in this particular nonequilibrium distribution.

6. Conclusion

In this article, I have tried to identify physical and mathematical properties that might be shared by both equilibrium and nonequilibrium phase transitions, the latter being defined with reference to stationary states generated by dynamics that are not time-reversal symmetric. In equilibrium systems, we understand the importance of a competition between energy and entropy in shaping the phase behaviour; away from equilibrium, the proper macroscopic characterisation is unclear.
However, as I have shown, when the equilibrium theory of phase transitions is presented from the perspective of microscopic stochastic dynamics, one has a picture that applies equally well to nonequilibrium dynamical systems as long as two criteria are satisfied. First, the dynamics must be ergodic—a property held by many nonequilibrium dynamical models (but see below). We also require a macroscopic phase to be associated with a peak in the stationary distribution that grows in a prescribed way with the system’s volume. Some additional precision in the definition of this association and clarity regarding its necessity is required.

Nevertheless, quantitative results relating to the well-studied asymmetric exclusion process (ASEP) are encouraging. As shown here, the stationary distribution in the space of macroscopic order parameters of a related equilibrium model behaves roughly as described in Section 3. A study elsewhere [36] shows similar structures in the space of nonequilibrium current and density macrostates, indicating a robustness that is not immediately obvious. Another curiosity is that nonanalyticities in a rather abstractly-defined free energy reflect the physical nature of phase transitions, as evidenced by patterns of partition function zeros. This is not an isolated case, similar results having been established for a number of related models [34, 26]. Although this suggests an intimate relationship between equilibrium and nonequilibrium phase transitions, one should not rule out the possibility that these models have been amenable to such detailed study precisely because they possess this special feature.

Finally, we should outline some criticisms of the theory outlined in Section 4. Most obviously, the expression (11) seems overprescribed: if one has an equilibrium dynamics, evaluation of the determinant in (11) is likely to give a much more complicated expression than that obtained by summation of the Boltzmann factors. Although one does not expect such additional factors to contribute any nonanalyticities to the equilibrium free energy, there is a problem demonstrated by certain spin glass models [40]. Specifically, at a dynamic transition temperature, the lifetime of a metastable state diverges, precluding relaxation to the paramagnetic state that has a lower free energy. Since $Z$ as given here in Eq. (11) can be shown [19, 22] to be inverse to the product of relaxation times, one might expect nonanalyticities in $Z$ unrelated to static phase transitions to arise after all. More widely, the notion of a partition function in the presence of such ergodicity breaking is at best ill-defined.

To conclude with a more general remark, it is worth noting that in our effort to understand nonequilibrium dynamics, it has become traditional to specify ad hoc stochastic rules with little attention paid to such thermodynamical considerations as heat and work. A bridge between the two is provided by fluctuation theorems [41, 42] such as Crooks’ equality [43] that relates products of transition probabilities to dissipated work. This suggests that it might be possible to separate the potential differences (6) for an arbitrary process into conservative and nonconservative parts. However, since the distinction is to some extent arbitrary [44], it is unclear how physically meaningful such a procedure would be.

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