I. INTRODUCTION

Given a system of many macroscopic units driving one another dynamically through strongly interactive, possibly mutually competitive and stochastically applied rules, one is often interested in determining the temporal development of some macroscopic observable(s). In general this is a difficult task, normally impossible without approximation. However, when (i) the individual units are identical, (ii) the microscopic update rules are instantaneous, and (iii) there is no spatial dependency to the interaction rules, experience with extremal dominance in equilibrium physics suggests that solution in a closed form for an appropriate set of observables (or order parameters) becomes at least potentially feasible in the limit in which the number of units $N$ tends to infinity. Indeed, for simple enough units with uniform interaction rules, a closed autonomous dynamical equation can be obtained involving only a single order parameter. On the other hand, when the interaction rules are non-uniform and involve significant random character the situation is very non-trivial even for the case of range-free interactions. Nevertheless, we have been able to make major progress with such problems, using a combination of exact results and ansätze to obtain closed autonomous macroscopic flow equations whose solutions are in very good accord with the results of numerical simulations of the microdynamics and suggest procedures to tackle other analogous and extended problems. In this paper we spell out the philosophy and execution of this new approach and demonstrate its application to simple models of spin glasses and recurrent neural networks.
where
\[ h_i(\sigma) = \sum_{j \neq i} J_{ij} \sigma_j + \theta_i \quad (2) \]

and \( \beta^{-1} \) is a measure of the degree of stochasticity. With appropriate coarse-graining this leads to the master equation for the microstate distribution \( p_t(\sigma) \)

\[
\frac{d}{dt} p_t(\sigma) = \sum_{k=1}^{N} \left[ p_t(F_k \sigma) W_k(F_k \sigma) - p_t(\sigma) W_k(\sigma) \right] \quad (3)
\]

where \( F_k \) is the spin-flip operator

\[
F_k \Phi(\sigma) = \Phi(\sigma_i, ..., -\sigma_k, ..., \sigma_N), \quad (4)
\]

\( W_k(\sigma) \) is the transition rate

\[
W_k(\sigma) = \frac{1}{2} \left[ 1 - \sigma_k \tanh(\beta h_k(\sigma)) \right], \quad (5)
\]

and we are now using the vector notation \( \sigma = (\sigma_1, ..., \sigma_N) \).

From (3) we may derive an equation for the evolution of the macrovariable probability distribution

\[
P_t[\Omega] = \sum_{\sigma} p_t(\sigma) \delta[\Omega - \Omega(\sigma)]; \quad \Omega \equiv (\Omega_1, ..., \Omega_n) \quad (6)
\]

in the form

\[
\frac{d}{dt} P_t[\Omega] = \sum_{\ell \geq 1} \frac{(-1)^{\ell}}{\ell!} \sum_{k_1=1}^{n} \ldots \sum_{k_\ell=1}^{n} \frac{\partial^\ell}{\partial \Omega_{k_1} \ldots \partial \Omega_{k_\ell}} P_t[\Omega] F_{k_1 \ldots k_\ell}[\Omega, t] \quad (7)
\]

where

\[
F_{k_1 \ldots k_\ell}[\Omega, t] = \langle \sum_{j=1}^{N} W_j(\sigma) \Delta_{j k_1}(\sigma) \ldots \Delta_{j k_\ell}(\sigma) \rangle_{\Omega, t} \quad \Delta_{j k}(\sigma) \equiv \Omega_k(F_j \sigma) - \Omega_k(\sigma) \quad (8)
\]

and the notation \( \langle \rangle_{\Omega, t} \) refers to a sub-shell average

\[
\langle f(\sigma) \rangle_{\Omega, t} = \frac{\sum_{\sigma} p_t(\sigma) \delta[\Omega - \Omega(\sigma)] f(\sigma)}{\sum_{\sigma} p_t(\sigma) \delta[\Omega - \Omega(\sigma)]} \quad . \quad (9)
\]

In several cases of interest and for finite times only the first term on the right hand side of (8) survives in the limit \( N \to \infty \), yielding the deterministic flow

\[
\frac{d}{dt} \Omega_t = \langle \sum_{i} W_i(\sigma) [\Omega(F_i \sigma) - \Omega(\sigma)] \rangle_{\Omega, t} \quad . \quad (10)
\]

In general this does not yet constitute a closed set of equations due to the appearance of \( p_t(\sigma) \) in the sub-shell average. However, we may attempt to find an appropriate choice of \( \Omega \) for which closure may be attained either exactly or approximately. Thus is done below for certain model systems.
III. SPECIFIC SYSTEMS

One particularly simple example occurs for the case of an infinite range Ising ferromagnet in a uniform external field; $J_{ij} = J_0/N$, $\theta_i = \theta^{ext}$. In this case the magnetization $m = N^{-1} \sum_i \sigma_i$ suffices alone as a macrovariable whose evolution is deterministic and closed,

$$\frac{d}{dt} m = \tanh(\beta(J_0m + \theta^{ext})) - m,$$

and yields the usual mean field solution in the steady state limit

$$\frac{d}{dt} m = 0 \quad \rightarrow \quad m = \tanh(\beta(J_0m + \theta^{ext})).$$

A greater challenge is posed by problems with sufficient disorder and frustration, such as those given by

$$J_{ij} = J_o/N + J z_{ij}/\sqrt{N}; \quad \langle z_{ij} \rangle = 0 \quad \langle z_{ij}^2 \rangle = 1; \quad i \neq j.$$  

where $z_{ij}$ is a quenched random parameter. This is the case for two particular model problems of interest on which we shall concentrate: the Sherrington-Kirkpatrick (SK) spin glass and the Hopfield neural network. In the SK model the $\{\sigma\}$ represent true magnetic spins and the $\{J_{ij}\}$ are chosen randomly from a Gaussian distribution. In the Hopfield model the $\{\sigma\}$ represent states of McCulloch-Pitts neurons, $\sigma = +1/-1$ corresponding to firing/non-firing, and the $\{J_{ij}\}$ provide for the storage and retrieval of random patterns $\{\xi \}$; $\mu = 1...p = \alpha N$, via the Hebb rule $J_{ij} = N^{-1} \sum_{\mu=1}^p \xi_i^\mu \xi_j^\mu$. Concentrating for simplicity on the region of phase space within the basin of attraction of one pattern, $\mu = 1$, it is convenient to apply the gauge transformation $\sigma_i \rightarrow \sigma_i \xi_i^1$. $J_{ij} \rightarrow \xi_i^1 \xi_j^1 J_{ij}$, $\theta_i \rightarrow \xi_i^1 \theta_i$ to re-write this in the form of (13) with

$$z_{ij} = \frac{1}{\sqrt{p}} \sum_{\mu>1}^p \xi_i^\mu \xi_j^\mu \quad J_o = 1 \quad J = \sqrt{\alpha} \quad \langle \xi_i \rangle = 0.$$  

In both cases we shall take $\theta^{ext} = 0$ for simplicity in this note. It is straightforward to show that $m = N^{-1} \sum_i \sigma_i$ is insufficient for a closed macroscopic evolution for finite $J$, although it does suffice if $J \rightarrow 0$ as $N \rightarrow \infty$, as is the case for a Hopfield model with only one condensed pattern, storing only a less than extensive number of patterns ($\lim_{N \rightarrow \infty} \alpha = 0$).

But how many macrovariables does one need and what are they? Before giving an answer to the last question which we believe to be at least very close to the truth, let us consider an intermediate step which is useful illustratively. Although our analysis applies to finite times, it is instructive to ask first about the long time steady state. For problems with detailed balance in their dynamics one knows that in the limit as $t \rightarrow \infty$ before $N \rightarrow \infty$ the microstate distribution takes the Boltzmann form $p_\infty(\sigma) \sim \exp(-\beta H)$. This is the case in the above examples which have $J_{ij} = J_{ii}$, yielding the Hamiltonian

$$H/N = -N^{-1} \sum_{i<j} J_{ij} \sigma_i \sigma_j = \frac{1}{2} J_0 m^2(\sigma) - J r(\sigma) + 0(N^{-1})$$  

where

$$r(\sigma) = N^{-3/2} \sum_{i<j} \sigma_i z_{ij} \sigma_j.$$  

Thus, as long as $r(\sigma) \sim O(1)$ it cannot be ignored in the set of $\Omega$. It is straightforward to show that $r(\sigma) \sim O(1)$ for both the SK spin glass and the Hopfield model at finite storage ratio $\alpha$. Thus we shall first discuss an attempt to find a non-equilibrium macrodynamics in terms of $m, r$, alone, and show that it provides a reasonable but imperfect description. We shall then go on to a more sophisticated theory in terms of a generalized order function which provides a very good fit to the results of microscopic simulation.
IV. THE SIMPLE VERSION OF THE THEORY: TWO ORDER PARAMETERS

In this section we choose the minimal form

\[ \Omega'(\sigma) \equiv (\Omega_1(\sigma), \Omega_2(\sigma)) = (m(\sigma), r(\sigma)). \]  \tag{17} \]

The resultant \( P_t[\Omega'] \) does indeed satisfy a Liouville equation in the thermodynamic limit, yielding the deterministic flow equations

\[ \frac{dm}{dt} = \int dz D_{m,r,t}(z) \tanh(\beta J_o m + J z) - m \] \tag{18} \]

\[ \frac{dr}{dt} = \int dz D_{m,r,t}(z) z \tanh(\beta J_o m + J z) - 2r \] \tag{19} \]

where \( D_{m,r,t}(z) \) is the sub-shell averaged distribution of the disorder contributions to the local fields

\[ D_{m,r,t}(z) = \lim_{N \to \infty} \frac{\sum_{\sigma} p_t(\sigma) \delta(m - m(\sigma)) \delta(r - r(\sigma)) N^{-1} \sum_i \delta(z - z_i(\sigma))}{\sum_{\sigma} p_t(\sigma) \delta(m - m(\sigma)) \delta(r - r(\sigma))} \] \tag{20} \]

\[ h_i(\sigma) = J_o m(\sigma) + J z_i(\sigma) + 0(N^{-1}) \quad z_i(\sigma) = N^{-1/2} \sum_j z_{ij} \sigma_j. \] \tag{21} \]

As yet, because of the \( p_t(\sigma) \) in (17), equations (18) and (19) are not closed except in the disorder-free case \( J = 0 \). To close the equations we introduce two simple ansätze: (i) we assume that the evolution of the macrostate \((m, r)\) is self-averaging with respect to the specific microscopic realization of the disorder \( \{z_{ij}\} \), (ii) as far as evaluating \( D(z) \) is concerned we assume equipartitioning of the microstate probability \( p_t(\sigma) \) within each \((m, r)\) shell. The first of these ansätze is well borne out by computer simulations of the microscopic dynamics and permits averaging \( D(z) \) over pattern choices. The second, which is clearly true as \( t \to \infty \) since \( p_\infty(\sigma) \) depends only on \( m \) and \( r \) but can only be judged \textit{a posteriori} for general time, eliminates memory effects beyond their reflection in \( m, r \) and removes explicit time-dependence from \( D \). Together these ansätze give

\[ D_{m,r,t}(z) \to D_{m,r}(z) = \left\{ \frac{\sum_\sigma \delta(m - m(\sigma)) \delta(r - r(\sigma)) N^{-1} \sum_i \delta(z - z_i(\sigma))}{\sum_\sigma \delta(m - m(\sigma)) \delta(r - r(\sigma))} \right\}_{\{z_{ij}\}} \] \tag{22} \]

where \( \langle \cdots \rangle_{z_{ij}} \) indicates an average over the quenched randomness. This yields closure of (18) and (19) since \( D_{m,r}(z) \) now depends only upon the instantaneous values of \( m, r \) and no longer on other microscopic measures of history.

The actual evaluation of \( D_{m,r}(z) \) from (22) remains a non-trivial exercise, but one which is amenable to solution by replica theory as developed for the investigation of local field distributions in spin glasses [4]. After several manipulations it can be expressed in the form

\[ D_{m,r}(z) = \lim_{n \to 0} \int \prod_{i,j} \prod_{\alpha,\beta=1...n} dx_i^\alpha dx_j^\beta \exp[-N \Phi(m, r, z; \{x^\alpha_i\}, \{y_j^{\alpha\beta}\})] \] \tag{23} \]

where the number of indices \( i, j \) is finite and \( \Phi \) is \( O(N^0) \). Because the argument of the exponential scales as \( N \), the integral can be evaluated by steepest descents.

The extremization is complicated [3,4] and in its complete form involves significant subtleties, including an extension of those devised by Parisi for the analysis of the spin glass problem.
It is discussed in detail elsewhere \[7,8\]; here we note only a few salient results. Important among them is that in the steady state limit of $\frac{dm}{dt} = \frac{dr}{dt} = 0$ the analysis yields the full thermodynamic results obtained from equilibrium analysis \[1\], including replica-symmetry breaking \[5\]. For more general times explicit analysis to date has only been completed within the further ansatz of replica-symmetry in the dynamic analogue of the spin glass order parameter $q^{\alpha\beta}$ which enters into the evaluation of $D_{m,r}(z)$, but including a determination of the limit of its applicability against small replica-symmetry breaking fluctuations (cf. \[10\].

The full analytic results for this case can be found in \[7,8\]. Here we simply exhibit graphically the comparisons between theory and microscopic simulation for the Hopfield model for $\alpha = 0.1$ and deterministic microdynamics; similar results hold for arbitrary $\alpha$ and $T$. Fig 1 shows flows in $(m, r)$, with time implicit, and it is observed that the comparison is quite good (but not perfect); it also clearly shows the need for (at least) two order parameters. On the other hand, Fig 2, which shows the dependence of $m$ and $r$ on $t$, demonstrates that the theory misses a slowing-down effect seen in the simulations for non-retrieving situations (ie. ones in which $\lim_{t \to \infty} m(t) = 0$). One may further note that the slowing-down occurs before the system crosses the limit of replica-symmetry stability against small fluctuations, suggesting that its origin lies other than in the breakdown of the RS ansatz used in the evaluation of $D(z)$. Rather, one is driven to conclude that the problem lies in the loss of memory information inherent in the assumption of equipartitioning in the form used above. This implies that the set of $\Omega$ must be expanded beyond just $m$ and $r$, to include more microscopic effects.

**FIG. 1.** Macroscopic flow trajectories for a Hopfield model with storage capacity $\alpha = 0.1$ and deterministic microscopic dynamics ($\beta = \infty$); dots indicate simulations ($N = 32000$), solid lines indicate analytic RS theory. The outer dashed line is the boundary predicted by RS theory; the inner dashed line indicates the onset of instability against RS-breaking fluctuations, with stability on the side closer to the origin.
FIG. 2. Temporal dependence of the order parameters for a Hopfield model with storage $\alpha = 0.1$ and zero-temperature dynamics ($\beta = \infty$); dots indicate simulations ($N = 32000$), the other lines indicate RS theory shown with solid lines where stable, dashed lines where unstable. Time is measured in Monte Carlo steps per spin.

V. THE SOPHISTICATED VERSION OF THE THEORY: ORDER FUNCTION DYNAMICS

To improve on the theory as developed in the last section requires broadening the range of order parameters. Addition of a finite number of extra observables, although technically relatively straightforward to effectuate, is not however expected to give more than just minor improvements; rather, a qualitative change of philosophy would seem to be required. To this end we propose instead for $\Omega$ the joint spin-field distribution

$$D(\varsigma, h; \sigma) = \frac{1}{N} \sum_i \delta_{\varsigma, \sigma_i} \delta \left[ h - h_i(\sigma) \right].$$

Our motivation for this choice is the following

1. The previous two dynamic parameters $m(\sigma)$ and $r(\sigma)$ can be written as moments off $D(\varsigma, h; \sigma)$, so the advanced theory automatically inherits the exactness in the two solvable limits $t \to \infty$ and $J \to 0$.

2. The order parameter function $D(\varsigma, h)$ specifies the underlying states $\sigma$ to a much higher degree than $(m, r)$; i.e. more microscopic memory is taken into account.

3. The microscopic equation (3) itself is formulated in terms of spins and fields.

4. The choice (24) allows for immediate generalization to models without detailed balance and to soft-spin models.
Strictly, $D$ is infinite-dimensional through $h$ in the limit $N \to \infty$, but in practice we expect it to be quasi-continuous and well-behaved (smooth). Hence we assume that we can evaluate it at a number $\ell$ of field values $h_\mu$ and take the limit $\ell \to \infty$ after the limit $N \to \infty$. We then have $2\ell$ macrovariables $\Omega_{\mu}(\sigma) = D(\zeta, h_\mu; \sigma)$, with $\mu = 1, \ldots, \ell$ and $\zeta = \pm 1$.

We may consider the distribution

$$P_t[D(\zeta, h)] = \sum_{\sigma} p_t(\sigma) \delta[D(\zeta, h) - D(\zeta, h; \sigma)]$$  \hspace{1cm} (25)

and analyze its evolution in a manner analogous to that applied earlier to $P_t(m, r)$. For finite $\ell$ it is again found to satisfy a Liouville equation for finite $t$ and $N \to \infty$, resulting in deterministic evolution of $D_t(\zeta, h)$. As before, this equation is not a priori closed since it involves expressions of the form

$$\langle f(\sigma) \rangle_{D,t} = \frac{\sum_{\sigma} p_t(\sigma) f(\sigma) \prod_{\delta,\sigma} \delta \left[ D(\zeta, h_\mu) - \frac{1}{N} \sum_j \delta_{\zeta,\sigma,j} \delta [h_\mu - h_j(\sigma)] \right]}{\sum_{\sigma} p_t(\sigma) \prod_{\delta,\sigma} \delta \left[ D(\zeta, h_\mu) - \frac{1}{N} \sum_j \delta_{\zeta,\sigma,j} \delta [h_\mu - h_j(\sigma)] \right]}$$  \hspace{1cm} (26)

where $p_t(\sigma)$ again implies knowledge of the full microstate distribution. Again, to achieve closure, we apply our two anzätze of self-averaging and equipartitioning, but in this case the latter is far less questionable since it assumes only that all microstates with the same distribution $D(\zeta, h)$ contribute equally (and not all states with the same two moments of that distribution $m$ and $r$). After some manipulation we obtain the relatively simple closed evolution equation

$$\frac{\partial}{\partial t} D_t(\zeta, h) = \frac{1}{2} [1 + \tanh(\beta h)] D_t(-\zeta, h) - \frac{1}{2} [1 - \tanh(\beta h)] D_t(\zeta, h)$$

$$+ \frac{\partial}{\partial h} \left\{ D_t(\zeta, h) [h - \theta - J_0(\tanh(\beta H)) D_t] + A[\zeta, h; D_t] + J^2 [1 - (\sigma \tanh(\beta H)) D_t] \frac{\partial}{\partial h} D_t(\zeta, h) \right\}$$  \hspace{1cm} (27)

with

$$A[\zeta, h; D_t] = - \lim_{N \to \infty} \frac{J}{N \sqrt{N}} \sum_{i \neq j} \langle \{z_{ij} \tanh(\beta h_j(\sigma)) \delta_{\zeta,\sigma,j} \delta [h - h_j(\sigma)] \} \rangle_{D_t}$$  \hspace{1cm} (28)

and

$$\langle \langle f(\sigma, H) \rangle_D \rangle = \sum_{\sigma} \int dH f(\sigma, H) D(\sigma, H)$$  \hspace{1cm} (29)

and

$$\langle \langle f(\sigma; \{z_{kl} \}) \rangle_D \rangle = \lim_{n \to 0} \sum_{\sigma_1} \cdots \sum_{\sigma_n} \langle f(\sigma_1; \{z_{kl} \}) \prod_{\alpha=1}^n \prod_{\delta,\mu} \delta \left[ D(\zeta, h_\mu) - \frac{1}{N} \sum_j \delta_{\zeta,\sigma,j} \delta [h_\mu - h_j(\sigma)] \right] \rangle_{\{z_{kl} \}}$$  \hspace{1cm} (30)
FIG. 3. Evolution of the binding energy of the Sherrington-Kirkpatrick spin glass ($J_0 = 0$) from a random microscopic start. Comparison of simulations ($N = 8000$, solid line) and predictions of the simple two-parameter ($m, r$) theory of section IV (RS stable, dotted; RS unstable, dashed) and of the advanced order-function theory of section V (solid), for $\beta = \infty$. Note that the two solid lines are almost coincident.

FIG. 4. Field distributions $D_t(\sigma,h)$ in the $J = 1$ SK model at $T = 0$, for $J_0 = 0$ (left) and $J_0 = 1$ (right). Histograms: numerical simulations with $N = 8000$; lines: result of solving the RS diffusion equation.
Replica theory can again be employed to determine the averages (30) to yield a closed autonomous equation for $D_t(\varsigma, h)$, although explicit numerical solution still involves the solution of a set of complicated saddle point equations; for details see [11]. To date we have only performed the evaluation within the RS ansatz. Results for the case of an SK model with $J_0 = 0$ are exhibited graphically in Figs 3 and 4, together of microscopic simulation and, in Fig 3 of the simpler theory of Section IV. It may be noted that the advanced theory is in good accord with the simulations, quite convincingly describing the transients of the simulation experiment, including the hitherto unexplained slowing down. Equally good fits for $D_t(\sigma, h)$ are obtained at finite temperature (11).

Replica-symmetry breaking analysis remains to be performed for arbitrary $t$, but we note that the difference in the asymptotic limit $t \to \infty$ is known from equilibrium theory where replica-symmetric theory gives $r_{RS}(\infty) = 0.798$, while the full replica-symmetry breaking theory gives $r_{RSB}(\infty) = 0.763$, the difference between which is very small on the scale of Fig 3.

VI. BEYOND DETAILED BALANCE

The sophisticated version of our theory, as discussed in the last section, does not make use of detailed balance and in (21) $h_i(\sigma)$ is simply given by (2), irrespective of the relationship between $J_{ij}$ and $J_{ji}$. The analysis goes through as in (24) to (30) even for more general choices of $z_{ij}$ not necessarily equal to $z_{ji}$. To illustrate its efficacy we have compared calculations and simulations for the case of an antisymmetric SK model with $z_{ij} = -z_{ji}$ with the $z_{ij}; j \neq i$ independently Gaussian distributed, with good agreement both at zero and finite temperature; we illustrate the results for $T = 0$ dynamics in Figs 5 and 6.

FIG. 5. Magnetization $m$ and energy per spin $E$ in the asymmetric $J = 1$ SK model at $T = 0$, for $J_0 = 0$ (left) and $J_0 = 1$ (right). Solid lines: numerical simulations with $N = 5600$; dotted lines: result of solving the RS diffusion equation.
VII. GENERALIZATIONS

So far we have considered only binary-valued microvariables. However, the treatment above can be extended to more general microvariables $\vec{S}_i$, where the overarrow denotes a low-dimensional vector$^1$, governed by some more general master equation for $p_t(\vec{S})$. If we continue to restrict to situations in which the instantaneous dynamics of $\vec{S}_i$ is determined, possibly stochastically, by a local force $\vec{F}_i(\vec{S})$ then the natural extension of the order function of section V is

$$D(\vec{S}, \vec{F}; \vec{S}) = \frac{1}{N} \sum_i \delta(\vec{S} - \vec{S}_i) \delta(\vec{F} - \vec{F}_i(\vec{S}))$$

(31)

An equation of motion for

$$\mathcal{P}(D(\vec{S}, \vec{F})) = \sum_{\vec{S}} p_t(\vec{S}) \delta[D(\vec{S}, \vec{F}) - D(\vec{S}, \vec{F}; \vec{S})]$$

(32)

may be generated as discussed above and in appropriate limits of time and size can be expected to lead again to deterministic flows for $D(\vec{S}, \vec{F})$. These in turn will in general involve force-fluctuation analogues of the noise distribution (20) and can in turn be closed via self-averaging and equipartitioning ansätze. We shall not, however, consider this more explicitly here.

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$^1$as opposed to the bold notation which indicates an $N$-dimensional vector
It may or may not be that a macroscopic observable of interest can be obtained from $\mathcal{D}(\vec{S}, \vec{F})$ alone. If this is not the case the order function must be expanded to allow for their evaluation.

VIII. CONCLUSION

We have demonstrated that for problems with instantaneous microscopic update dynamics, which may involve both quenched and stochastic randomness provided that the interactions are drawn from range-free distributions, one can derive closed autonomous deterministic dynamics for appropriately chosen order parameters, in good accord with simulations for examples studied. In principle, extensions to finite-range interactions could be considered but would involve greater approximation.

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