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Final Report

STUDIES OF SPATIAL AND TEMPORAL DISORDER IN MACROSCOPIC SYSTEMS

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I. Introduction

This document constitutes the final report of research conducted under the DOE grant "Studies of Spatial and Temporal Disorder in Macroscopic Systems".

There are three sections to this report, each describing research in a different general area, and a bibliography consisting of published journal articles reporting that research.

This grant has no unexpended funds.

II. The Weak-Noise Characteristic Boundary Exit Problem

In the initial phase of this project, we developed a systematic treatment of the generic weak-noise escape problem, when exit from the domain of attraction occurs preferentially near a saddle point.

Our approach to the limit of weak noise ($\epsilon \rightarrow 0$) is one of matched asymptotic expansions. We studied the principal eigenfunction of the Fokker-Planck operator (i.e., the quasistationary probability density), and approximated it by a characteristic (ray) expansion. These rays are zero-energy Wentzell-Friedlin trajectories, whose action $W(x)$ (sometimes called the nonequilibrium potential governs the exponential suppression of noise-induced fluctuations away from the stable point S . In physical terms, the characteristic expansion is an asymptotic WKB expansion of the quasistationary density. Our expansion turns out to be generated by a system of ordinary differential equations, which must be integrated along the rays. Because our method requires the solution of ordinary differential equations, it is easier

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to implement than those proposed in earlier works; in particular, it is better suited to numerical computation than these earlier methods. In later papers we generalized our method and presented a set of fully covariant equations, which transform systematically under changes of coordinates. We showed that a key role in the computation of an asymptotic expansion for the quasistationary probability density is played by a Riccati equation for the matrix of second derivatives of the action W , and provided a geometric, coordinate-free interpretation of our results.

One of our most important early results concerns the weak-noise asymptotics of the MFPT, which we were able to estimate in terms of the rate at which probability is absorbed on the boundary of the domain of attraction. We found that the standard Eyring formula for the MFPT fails for the general nongradient case, which is not in itself surprising. What *is*, perhaps, surprising is that we showed that *no formula analogous to the Eyring formula even exists*, in that the pre-exponential factor in the MFPT (while still independent of ϵ) now depends on the drift field and its derivatives *everywhere* in the vicinity of the MPEP between the stable point S and the saddle point. That is, the $\epsilon \rightarrow 0$ formula for the MFPT is now *nonlocal* in the drift.

This does not seem to have been widely appreciated prior to our work. It can be viewed as an example of the “Blowtorch Theorem” discussed by Landauer and others, most often in the context of one-dimensional models with multiplicative noise. Our results indicate that it is very likely a general consequence of the absence of detailed balance.

We also investigated the dynamics of escape attempts, and found that, in contrast to the gradient case, the ‘optimal’ (most probable) noise-induced fluctuational paths are not in general anti-parallel to incoming deterministic trajectories. So each unsuccessful escape attempt is in general a closed *loop*; circulation is present even on the shortest length- and time-scales.

Finally, we noted that outgoing optimal trajectories can cross, forming *caustics* of a sort familiar from geometrical optics, and giving rise to a new array of previously unexplored phenomena. That caustics can occur in the flow pattern of the most probable fluctuational paths has been known for some time, but our work was the first to consider the effects on exit phenomena. On a caustic, the nonequilibrium potential $W(x)$ is nondifferentiable. If a caustic appears near an exit point, new phenomena will arise.

The presence of caustics profoundly affects exit phenomena. While most modifications of the Eyring formula discovered up to now, for nongradient drifts, affect the subdominant weak-noise asymptotics of the MFPT (i.e., its pre-exponential factor), here we find that the *leading-order* asymptotics are changed; that is, the presence of caustics near the exit point affects the *exponential dependence of the MFPT on the noise strength*. The literature often states that finding the leading-order asymptotics of the MFPT is not a difficult or subtle problem; the far greater difficulty is in computing the prefactor. We see here, however, that for nongradient drift fields, extreme care must be used in computing even the leading-order asymptotics!

We subsequently performed a comprehensive analysis of the exit distribution problem when escape as $\epsilon \rightarrow 0$ is increasingly concentrated about a saddle point. We showed,

using formal methods, that the asymptotic form of the exit location distribution on $\partial\Omega$ is *generically* non-Gaussian and asymmetric (or skewed).

That skewing can occur was first pointed out by Bobrovsky and Schuss; some recent rigorous results were obtained by Bobrovsky and Zeitouni, and by Day. However, the phenomenon has until now remained unclarified; the first explicit examples of skewed asymptotic exit distributions were given in our paper on caustics. We also showed that skewing is a generic phenomenon, and derived a general result, analogous to the central limit theorem, which characterizes skewing: in any generic stochastic exit model, of the type described above, with characteristic boundary, the exit location distribution will be asymptotic to a non-Gaussian distribution (on an appropriate ϵ -dependent lenscale near H) that belongs to one of two well-defined classes.

We then built on previous work by analyzing the bifurcation phenomenon which appears at the onset of a caustic. This new phenomenon is a bifurcation of the most probable transition path (in the limit of weak noise) between the two wells of a double-well model, as a system parameter is varied.

In many ways, the behavior of a system whose most probable transition path is just beginning to bifurcate resembles that of a system undergoing a *phase transition*. For example, a qualitative change in the behavior of the most probable fluctuational trajectories will occur. Another indication is in the WKB prefactor, which determines the prefactor of the mean first passage time; in our work we showed that it diverges at the transition point.

As a consequence, double well systems which are 'at criticality' in the bifurcation sense will exhibit non-Arrhenius behavior. This means that the growth of the mean time between inter-well fluctuations, i.e., the growth of the mean time needed for the system to hop from one well to the other, will *not be pure exponential* in the weak-noise limit. In double well systems at criticality, relaxation due to activation will proceed (in the limit of weak noise) at an anomalous, in fact anomalously large, rate.

In recent work, we began an international collaboration with groups in England and Italy to test our theoretical work, and also to uncover new avenues for exploration. An electronic analog model of our model system was built, and its output analyzed with a digital data processor. Complementary digital simulations were carried out. In both cases optimal fluctuational and relaxational trajectories were generated, and first passage times and exit location distributions were measured. Good agreement with our theoretical predictions was found.

Further experimental insight into the character of broken symmetry for the MPEP was gained by following relaxational trajectories, in order to obtain a complete history of the time evolution of noise-induced fluctuations away from the vicinity of the stable point. A clear signature of broken time-reversal symmetry was found; also, the prediction of closed trajectory loops for *unsuccessful* escape attempts was also verified. These results do more than confirm our earlier theoretical predictions: the results may also bear on two-dimensional stochastic ratchets where symmetry plays an important role.

III. Spin Glasses and Other Systems with Quenched Disorder

While much of the theoretical work on spin glasses has focused on the EA model or its infinite-ranged counterpart, other classes of models are also of interest. Among the most important are models with random long-ranged interactions that are square-summable (for example, that decay as a power law).

We studied such models and proved a number of surprising results, such as the following. With probability one, there exist *uncountably many* infinite volume ground states $\tilde{\sigma}$ that have the following unusual property: for *any* finite temperature, there is a Gibbs state supported entirely on infinite-volume spin configurations that differ from $\tilde{\sigma}$ only at *finitely* many sites. These results are examples of the bizarre effects that can occur in disordered systems with coupling-dependent boundary conditions. This insight proved to be useful in later studies, in particular our work on metastates.

In other work, we considered the issue of multiplicity of states in nearest-neighbor models, employing a new strategy in order to clarify some of the issues surrounding this controversy. We introduced a new spin glass model designed to clarify the relation between disorder and frustration on the one hand and multiplicity of ground states on the other. The model was chosen for its mathematical tractability rather than for physical realism. However, the results are suggestive, and definitively settle one issue that has caused a great deal of confusion in the literature: that is the claim that disorder and frustration are either necessary, or sufficient, or both, in order for a system to possess many ground states. Our results make it clear that the joint presence of disorder and frustration alone is not sufficient to draw any *a priori* conclusions about ground state multiplicity.

More interestingly, we demonstrated that our model has a *transition* at eight dimensions: in lower dimensions it possesses only a single pair of ground states in the thermodynamic limit, while above eight dimensions it has uncountably many. (Our methods do not reveal what happens exactly *at* eight dimensions.) Moreover, the mechanism by which the number of ground states changes can be precisely identified. This is the first example of a short-ranged spin glass model, with nontrivial ground state structure, which allows for an explicit computation of the number of ground states.

Of equal interest is that we found a mapping of our model to invasion percolation, and simultaneously addressed a problem in that field; namely, the question of whether one or infinitely many invasion regions exist in d dimensions. It should be noted that although the relation between multiplicity of ground states and multiplicity of invasion regions is exact and rigorous for all d , the solution of the invasion multiplicity problem has been carried out with complete rigor only for $d = 2$.

The work on multiple ground states and invasion percolation led us to some subsequent research in an unanticipated direction, but one which could eventually have consequences for understanding the dynamics of disordered systems. It also connects to a basic problem, of general mathematical interest. This is the problem of a *random walk or diffusion in a random environment*. We examined the low-noise limit of this problem so as to extract

some global information about *all* the transitions undergone over all time. Since the various transitions occur on exponentially different timescales, this cannot be done by observing the process directly, for any scaling of time. Our strategy instead was to observe *the order in which transitions are made for the first time*. We proved that invasion percolation arises as a low-noise (or high-disorder) limit of a general class of random walks in random environments (RWRE's).

This result has an interesting application to problems whose dynamical behavior can be modeled through the time evolution of random walks on "rugged landscapes", where ergodicity is broken on observable (and often far longer) timescales. Our analysis demonstrated that some of the central assumptions of broken ergodicity which are largely based on one-dimensional pictures, don't hold (at least in RWRE models) in higher dimensions. For example, components (that is, regions where the system is confined on fixed timescale) are usually assumed to be bounded; however, in our models they correspond to the invasion regions, which are infinite in extent. More importantly, previous analyses have assumed that on any timescale, the system is confined by a free energy barrier which grows logarithmically with time. While we find that this assumption is true in one dimension, it fails in higher dimensions; simply put, the system can get around high barriers. In fact, the invasion picture leads to the conclusion that confining barriers actually *decrease* as time progresses. Finally, in the usual pictures of broken ergodicity, the system returns infinitely often to previously explored regions of state space during the diffusion process. We found, however, that viewed on a sufficiently large scale the system does *not* return to previously explored regions of state space.

We then examined some experiments on irreversibility and aging in spin glasses, and applied these ideas to their interpretation. We found that some experimental results are more naturally interpreted within our framework than the standard one.

Our analysis demonstrates a surprising degree of emergent structure from what appears initially to be a rather featureless landscape. Our hope is that our work will lead to treatments of increasingly complex models, with a continual refinement of our understanding of how spin glasses and other disordered systems break ergodicity. We hope to apply the insights gained from this study to problems in biological evolution and in algorithm efficiency.

Two fundamental problems in spin glasses are those of the existence of a thermodynamic phase transition for realistic (i.e., non-infinite-ranged) models, and (should such a transition occur) the structure and ordering of the low-temperature spin glass phase. Any meaningful comparison of theory to experiment requires an understanding of these central issues. Competing theoretical pictures of the spin glass phase in realistic models include an "SK picture", in which features of the Parisi solution of the infinite-ranged SK model are assumed to apply to non-infinite-ranged models, and the droplet/scaling picture of Fisher and Huse.

We rigorously ruled out the central features of the Parisi solution for short-ranged models, and presented a general picture of the allowable structure for the spin glass phase and its order parameter(s). This also clarified the relations among chaotic size dependence, replica symmetry breaking, overlap non-self-averaging, and other features (some new) of spin glasses.

These results rigorously demonstrate non-mean-field behavior for short-ranged spin glass

models, and in fact, our conclusions hold also for a wider class of models, including those with diluted RKKY interactions (for such models, however, there is no general theory of infinite volume states or their decompositions into pure phases). Hence the SK picture in its most straightforward interpretation cannot be valid. One question is then whether and how any aspects of mean-field behavior can survive in realistic spin glasses. We addressed this issue in our next paper, as part of our consideration of the more general question of how one approaches the thermodynamics of a system with many competing pure states. These considerations led us to the idea of the *metastate*.

In pursuing this further, we presented a novel approach to the competition between thermodynamic states in spatially inhomogeneous systems, such as the Edwards-Anderson spin glass with a fixed coupling realization. This approach, modelled on chaotic dynamical systems, led to a classification of the allowable structures for replicas and their overlaps.

Our proposal was based on an analogy with chaotic deterministic dynamical systems, where the chaotic motion along a deterministic orbit is analyzed in terms of some appropriately selected probability measure, invariant under the dynamics. Time along the orbit is replaced, in our context, by L and the state space (or configuration space or phase space) of the dynamical system is replaced by the space of Gibbs states (for a fixed $\mathcal{J}$). This leads to a limiting measure, even in the presence of CSD, but it is a measure on the thermodynamic states themselves. This (infinite-volume) measure contains far more information than any single thermodynamic state, and has a particular usefulness in the context of the study of the relation of finite volume Gibbs states to the overall thermodynamics of the system. In simpler systems this is usually not an issue, but our work has shown that, if many competing pure states exist, this relation can be highly subtle. The proper tool for its analysis would then be the metastate.

At the same time that we ruled out the “standard” SK picture, we also proposed a new picture that we called a “nonstandard” SK picture. Here, the metastate is dispersed over many separate thermodynamic states, each with a sum decomposition over pure states (as in the standard Parisi solution).

If any of the familiar features of the Parisi solution are to survive in short-ranged spin glass models, even in the strongly altered form described above, then something like this nonstandard SK picture must be present. However, in a very recent paper, we presented a combination of heuristic and rigorous arguments, based on the invariance of the metastate under changes between gauge-related boundary conditions, that indicate both the pure state structure and the overlap structure of realistic spin glasses should be simple: in any finite volume with coupling-independent boundary conditions, such as periodic, at most a pair of flip-related (or the appropriate number of symmetry-related in the non-Ising case) states will appear, and the Parisi overlap distribution will correspondingly be just a pair of δ -functions at $\pm q_{EA}$ (the Edwards-Anderson order parameter). This rules out the nonstandard SK picture, and when combined with our previous results ruling out more standard versions of the mean field picture, eliminates the possibility of even limited versions of mean field ordering in realistic spin glasses. If broken spin flip symmetry should occur, this leaves open two main possibilities for ordering in the spin glass phase: the droplet/scaling two-state

picture, and the chaotic pairs many-state picture introduced earlier.

IV. Dynamical Problems Arising From Protein Biophysics

For the past several years I have been involved in an ongoing collaboration with Walter Nadler (Theoretical Chemistry, University of Tübingen) to develop mathematical methods for the study of dynamical processes in proteins. Our research has focused chiefly on two related problems of biological importance. The first concerns understanding the process whereby a ligand (*e.g.*, O₂ or CO) diffuses through the protein matrix to reach the internal heme site in hemoglobin or myoglobin. The second relates to the development of quantitative methods for computing closing time distributions arising from ion channel fluctuations.

Ligand migration in globular heme proteins is a primary example of transport through protein matter facilitated by internal fluctuations. A large body of experimental work over the past 20 years has led to the identification of several stages of the binding process. The main steps are the entrance of the ligand from the solvent into the protein, diffusion of the ligand within the protein matrix until the heme group is reached, and subsequent binding at the heme site. At a physical and mathematical level of description, these processes remain poorly understood.

For these processes to occur, protein conformational fluctuations are crucial. Analysis of the conformational structure of myoglobin shows that no paths exist from the protein surface to the heme pocket when the protein is frozen into a static, average conformation. This was observed many years ago, in an experiment which used flash photolysis to separate the ligand from the heme site. It was found that when myoglobin within a glycerol-water solvent is cooled to below the solvent's glass transition temperature ($\approx 200^\circ K$), no ligand diffusion within the protein matrix is observed. Presumably, the solvent's glassy state freezes out conformational fluctuations of the protein.

Our primary concern has been to lay the mathematical foundations for a correct theoretical description of processes governed in whole or in part by protein conformational fluctuations; these include in particular ligand diffusion through a protein matrix, and passive ion channel transport. Work under this DOE grant has led to the construction and solution of several mathematical problems interesting in their own right.

During the first DOE grant period we largely completed an extensive treatment of ligand diffusion in globular proteins. Experimental studies of the diffusional part of the ligand binding process found that the number of unrecombined molecules $N(t)$ at time t after flash photolysis often decayed with a $t^{-1/2}$ law, crossing over to an exponential at longer times. Previous work utilized a single-channel hypothesis, which assumes that the ligand follows a one-dimensional path through the protein. However, the correctness of this assumption remained unclear, and it became important to determine the true dimensionality of the ligand path.

We modelled this situation by employing a straightforward d - dimensional reaction-

diffusion model with appropriate inner and outer boundary conditions to study diffusion within a protein matrix. The protein conformational fluctuations will renormalize the effective diffusion constant for this process; this was the subject of separate work, described below. Here we confined ourselves to studying the time-dependence of $N(t)$. In our model, the $t^{-1/2}$ law emerges naturally, as does the crossover to exponential decay. More importantly, for biologically realistic values of the model parameters (and a large range to either side) these time-dependences hold for a diffusional path of *any* dimension. However, we found a clear feature which distinguishes one-dimensional from higher-dimensional channels: in three (and higher) dimensions, a well-defined "plateau" in $N(t)$ should be clearly observable (and was probably observed, though not understood, some time ago). This work then provided a sharp experimental test to resolve the open question of dimensionality of the ligand path.

The second component of our work on this problem concerned diffusive transport in fluctuating media. It has long been recognized that ligand transport within globular proteins does not occur in a static environment. Diffusion within a fluctuating medium occurs in many other contexts, including ionic conduction in polymeric solid electrolytes and protonic diffusion in hydrogen-bonded networks. In globular proteins, the ligand cannot diffuse until a random conformational fluctuation opens a local channel in its vicinity. This raises the problem of transport in a medium that is *dynamically*, or temporally, disordered.

A correct treatment of ligand diffusion in the heme proteins must therefore take into account that local pathways for the ligand will appear and disappear randomly. Any attempt to make theoretical contact with temperature and/or pressure studies of ligand recombination in heme proteins must come to grips with this problem. We were therefore led to consider, as a first step, the problem of diffusion on a fluctuating lattice.

With David Levermore (Mathematics Department, University of Arizona), we therefore set out to devise a new quantitatively accurate treatment of this problem and to perform simulations to compare against our results. We devised a renormalization group procedure that, while valid in any dimension, is particularly easy to implement in one dimension.

Our method used the fact that if we rescale space and time appropriately, then both the diffusion relation and the equations governing the bond fluctuation dynamics remain invariant. Iteration of the ensuing transformation equations introduces a flow in the parameter space (p, τ) . Hence, starting from the bare model parameters (p, τ) , we iterated the renormalization group (RNG) transformations until a fixed point is reached. From this we obtain D_{eff} , which corresponds to the value p^* at the stable fixed point.

We then performed extensive Monte Carlo simulations of random walks on a fluctuating lattice in one and two dimensions. We found that agreement between theory and simulation was very good in the one-dimensional case when only a 2-step RNG procedure was carried out. Comparison with effective medium theories showed that the relative error is smaller everywhere for the RNG method, even in the 2-step case. Agreement can be improved by increasing the number of steps in the RNG calculation.

In higher dimensions our procedure, as it now stands, becomes cumbersome; the number of terms which must be computed in an n -step calculation rises extremely fast with

dimension, scaling as d^n . Moreover, it is necessary to use larger n as d increases, so that dimensional effects (e.g., closed loops) are seen. However, preliminary results from a 4-step calculation in two dimensions already show the proper trend.

Our renormalization group procedure is therefore the first treatment that shows promise for yielding an accurate quantitative treatment of the random walk on a fluctuating lattice. Moreover, it is not restricted to limited regions of parameter space or small fluctuations, as were previous treatments. It is presently practicable to use only in low dimension, however.

A different area of exploration concerned the ion channel problem, which is intimately related to protein conformational fluctuations. Within certain proteins, single passive channels are available for ion migration. These ion channels fluctuate between two states: open and closed. The closing time distribution in particular has been well studied and displays a $t^{-3/2}$ tail.

With my former graduate student, Tsongji Huang, we proposed and solved a new type of random walk problem in a high-dimensional space (which represents the configuration space of the protein). The new feature is that the space is randomly partitioned between two types of sites.

Consider a lattice in a d -dimensional space, where each point in the lattice is of type A (corresponding, for example, to the open state) with probability p and of type B (for example, the closed state) with probability $1 - p$. The probabilities are taken to be independent.

We now ask the following question: suppose that a particle is found at the edge of an open cluster at time zero, and subsequently executes a random walk. What is the probability $P(t)$ that at time t it remains within the same cluster?

This is the problem of a random walk on a randomly partitioned space (RWRPS). Aside from serving as a new approach towards a theory of protein fluctuations, this problem is also of mathematical interest, describing a new class of transport problems. We solved this problem exactly in one dimension in two different ways: through a standard eigenfunction expansion, and through a direct counting technique. The first of these is useful only in one dimension, but the second lends itself to higher-dimensional extensions. The expression for $P(t)$ is complicated and must be evaluated numerically for arbitrary p . Already in one dimension, $P(t)$ displays interesting dynamical behavior. For $p = 0$, we have simple single-exponential decay, as expected; and for $p = 1$, the long-time behavior of $P(t)$ is a power-law falloff. For $0 < p < 1$, however, we find an interesting dynamical behavior, where $P(t)$ exhibits relaxation that is slower than exponential but faster than power law.

In high dimensions the analysis becomes more difficult, due to the large number of lattice animals corresponding to even small clusters, and it is doubtful that an exact solution can be found. In our next step, we studied the RWRPS problem on a randomly partitioned *Bethe lattice*, or Cayley tree. The behavior exhibited here should be characteristic of what occurs in very high dimensions. The direct counting technique mentioned in the previous section allowed us to exploit the tree-like structure of the Bethe lattice, and the results gained from it matched well with numerical simulations.

We confined our attention in this paper to discrete time dynamics, which allows for a unified treatment of the problem on general lattices. We were able to reduce the problem to the

determination of a volume exploration structure function for random walks, under certain boundary conditions. The key idea is that this function is *independent* of the partitioning.

Using this method, we found that $\langle N(n) \rangle$ displays three types of behavior, depending on p and d : an exponential decay, a Kohlrausch-Williams-Watts stretched exponential law, and a power law.

Finally, we used these results to compute the closing time distribution, which is the physical observable usually measured in passive ion channel transport experiments. Because the state space of proteins is very high-dimensional, we used a Bethe lattice with $z = 3$; results on this lattice were indistinguishable from results on Euclidean lattices in large dimension. We found that the best fits to experiment occurred for p close to, but not equal to, one.

These projects have moved us closer to a mathematical theory of protein fluctuations relevant to both ligand diffusion and ion channel fluctuations. New and interesting mathematical problems are concurrently raised, and their solution led to some interesting new techniques.

V. PUBLICATIONS CREDITING DOE SUPPORT DURING THE PERIOD JUNE 1, 1993 – PRESENT

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23. “Equilibrium Pure States and Dynamical Chaos” , C.M. Newman and D.L. Stein, submitted to *Physical Review Letters*, 1998.

VI. GRADUATE STUDENTS RECEIVING PH.D.’S DURING GRANT PERIOD

In December, 1995, Tsongjiy Huang, a graduate student supported on this DOE grant, received his Ph.D. from the University of Arizona. Thesis title: “Random Walks on Randomly Partitioned Lattices with Applications Towards Protein Fluctuations”.