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Exact computations test stochastic Loewner evolution and scaling in glassy systems

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Quenched disordered systems are notoriously difficult to solve precisely, so reliable and efficient computational methods are critical for testing theoretical ideas. However, in most cases the computational complexity for finding exact global minima of quenched systems grows exponentially with increasing sample size. Nevertheless a valuable subset of quenched disordered systems may be solved using exact polynomial (P) algorithms [1, 2], including spin glasses in two dimensions [3], the random field Ising model [4], several rigidity percolation problems [5, 6], some interface [7] and path problems [8] in disordered media, and the glassy solid-on-solid models studied by Schwarz and co-workers [9]–[11]. In these cases computational studies are no longer haunted by metastability, enabling a careful analysis of key questions that are otherwise much more difficult to resolve. Using these methods, Schwarz and co-workers confront several challenging issues in glass physics, including the relevance of stochastic Loewner evolution (SLE) [12, 13], the scaling of droplet excitations and the characterization of static chaos.

The model used consists of an SOS model with random offsets, the random substrate model [10, 11, 14]. At each site of a square lattice there is a height variable h_i that consists of the sum of a quenched random substrate offset $d_i \epsilon [0, 1]$ and a non-negative integer n_i, such that $h_i = d_i + n_i$. The SOS energy is taken to be quadratic in the height differences, $\sum_{\langle ij \rangle} (h_i - h_j)^2$. This problem is glassy at low temperatures and is related to several problems, for example the sine–Gordon (SG) model with random phases. These models are often called periodic elastic media (PEM) due to the periodic nature of the sinusoidal function in the SG energy, and the fact that in the SOS model adding an integer to all of the

heights does not change the energy. At high temperatures the random substrate model is in the usual SOS rough phase so the roughness $w^2 \sim \ln L$ and the pair correlations grow logarithmically with distance $C(r) = \langle h(r)h(0)\rangle \sim \ln r$. However functional RG calculations showed that at low temperatures there is a so-called super-rough phase where $w^2 \sim (\ln L)^2$ and $C(r) \sim (\ln r)^2$. The low temperature properties are difficult to simulate using Monte Carlo methods, even when using advanced sampling algorithms such as replica exchange methods. The key advance for enabling precise computation of the low temperature properties of the model is through a mapping to a well-known polynomial (P) problem in computer science, the minimum cost flow problem [9].

In general, the minimum cost flow problem consists of a graph where each edge has a cost c_{ij} and we impose boundary conditions where a flow is injected at a set of source sites s_i and it is taken out at a set of target sites t_j [1, 2]. The optimization problem is to find flow paths to minimize the cost of the flow. Mapping of this problem to the SOS with random offsets is invoked by simply noting that $h_j - h_i = d_{ij} + x_{ij}$, where $x_{ij} = n_j - n_i$ and $d_{ij} = d_j - d_i$, and that the variables x_{ij} obey Kirchhoff's current conservation at each node of the dual lattice. Since the energy is also in terms of height differences it is natural to consider a new optimization problem $\sum_{ij}(d_{ij} + x_{ij})^2$, with the constraint of current conservation at each node of the dual lattice. The optimization is then with respect to the 'integer flow variables' x_{ij} on the dual lattice and the problem is of the form of the well-known minimum cost flow problem. The quadratic function in the energy can be replaced by any convex function, though in general the minimum cost flow problem with unbounded constraints is pseudo-polynomial rather than P.

For a given set of offsets, $d_{ij} = d_i - d_j$, the minimum cost flow calculation finds the set x_{ij} that minimizes the cost. It works by starting with a frozen configuration of d_i and an initial guess for n_i. Two conditions then have to be met: feasibility, which means that flow conservation is valid; and optimality, which means that the lowest energy flow has been found. If feasibility is ignored, optimality is easy to achieve, namely for all $-0.5 \leq d_{ij} \leq 0.5$ set $x_{ij} = 0$, while for all $d_{ij} > 1/2$, set $x_{ij} = -1$, and for $x_{ij} < -1/2$, set $x_{ij} = 1$. It is easy to see that this minimizes the cost function $\sum_{ij}(d_{ij} + x_{ij})^2$. Starting from this optimal solution we can then try to impose feasibility. This is achieved by finding the excess flow at each site in the optimal configuration, that is the degree to which feasibility is violated. The excess flow is removed by finding augmenting paths from sites with excess outflow to those with excess inflow, and then removing the flow on these paths. This leads to an increase of the cost; moreover the augmenting paths can be chosen to have minimum effect on the cost by using standard shortest path algorithms, such as Dijkstra's method that applies to cases where the costs are positive. The really nice result is that if optimal augmenting paths are added until the flow is feasible, the final result is the global minimum of the convex flow problem.

Domain walls can be imposed by fixing part of a sample boundary to be at height n_0 and another part to be at $n_0 + 1$, yielding domain walls with fractal dimension $d_s = 1.25 \pm 0.01$. If domain walls in two-dimensional systems are conformally invariant they are expected to follow stochastic Loewner evolution (SLE) [12] where a parameter κ characterizes the 'left-passage' probability of a path. In that case the relation $d_s = 1 + \kappa/8$ is expected. However, there is no reason to expect quenched disordered systems to be conformally invariant; nevertheless the authors of a recent calculation of domain walls in 2D spin glasses [13] suggest that SLE may apply. It is thus very interesting to

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question whether this is a general result or whether the 2D spin glass numerical result is coincidental. Schwarz and co-workers [11] test this question for the random substrate SOS model and find that domain walls in this problem have fractal dimension $d_s = 1.25$ while κ is either approximately 4 (periodic boundaries) or 3 (both ends of the domain wall free), so $d_s = 1 + \kappa/8$ is violated. They conclude that SLE does not appear to apply for their system.

An important general scaling relation in all areas of statistical physics is the energy required to create an excitation at length scale L, $\Delta E \approx L^{\theta}$, as a positive value of θ indicates a stable phase while a negative θ indicates low energy long-range excitations that can be activated even at low temperatures. In the random substrate SOS model, the calculation of ΔE consists of finding the change in the ground state energy when the central site is fixed to be $n_c + 1$, where n_c is the height of the center site in the ground state when the boundaries are at height n_0. If the droplet, defined by the compact domain containing the center site and having height equal to $n_c + 1$, lies entirely within a box of size L around the center, then it is a droplet excitation of size L. It is known that for this system, $\theta = 0$; however $\theta = 0$ allows for a variety of droplet scalings for $L \to \infty$, including $\Delta E \approx \ln L$, $\Delta E \approx \ln \ln L$, $\Delta E \approx$ const etc. Only the latter is compatible with the instability of the ground state against thermal fluctuations (i.e. absence of a $T = 0$ fixed point). The precise calculations of Schwarz *et al* show that $\Delta E \approx$ const for $L \to \infty$, so the glass phase is marginally stable, implying that the low temperature phase may have temperature dependent scaling exponents, as suggested in some theoretical calculations.

Static chaos refers to the sensitivity of some glass phases to small changes in either the temperature or other parameters in the problem. This is again quite easy to define in terms of minimum cost flow: a starting configuration of the offsets d_i is augmented by a random perturbation δd_i. Then it is checked whether the correlation function between the unperturbed and perturbed state, $C_{12}(r)$, is like that of the unperturbed state. Chaos occurs when $C_{12}(r)$ changes to a different, less correlated, scaling at long distances. In spin glasses chaos occurs on length scales $L > L_\delta$, where $L_\delta = \delta^{-1/\alpha_s}$, with $\alpha_s = d_s/2 - \theta$. In contrast, in the disordered SOS model $\alpha = d/2 - \theta$, so for $\theta = 0$ it is $d/2$. FRG calculations suggest that $C_{12}(r) \sim \sigma[\log(r)]^2$ [15] for $L < L_\delta$ and it is also suggested that $C_{12} \sim \hat{\sigma} \log(r)$ for $L > L_\delta$. However it is difficult to use FRG calculations to demonstrate the $L > L_\delta$ results or the value of $\hat{\sigma}$. The exact computations of Schwarz *et al* show that the scaling is indeed logarithmic for large $L > L_\delta$ and hence that $\hat{\sigma} > 0$, demonstrating that static chaos does occur in this model.

The incisive results achieved through use of exact P calculations of the random substrate SOS model motivate a search for other polynomial quenched random systems that may shed further light on the glass state. A perhaps surprising aspect is that although the random substrate SOS model is solvable in polynomial time, this problem, and other P problems, have many of the hallmarks of the glass state. This raises questions: What general aspects of glass physics are only contained in hard computational problems, and what aspects are fully captured by P problems? In particular, do NP-complete problems have any generic glass features that are not present in P problems?

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