Application of exact combinatorial optimization algorithms to the physics of disordered systems

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Abstract

We discuss various applications of exact combinatorial optimization methods in the statistical physics of disordered systems. The physical systems we consider are elastic manifolds and elastic media with and without periodic potential. The algorithms we use find the exact ground states of these systems in polynomial time and allow for a thorough finite size scaling analysis that give accurate results for the universal properties, i.e. in particular critical exponents, of these systems.

Key words: Disordered systems, Ground states, Combinatorial Optimization
PACS:

1 Introduction

The physical properties of solid materials which contain a substantial degree of quenched disorder, so called disordered systems, have been an experimental and a theoretical challenge for many decades. The different thermodynamic phases emerging in random magnets, the aging properties and memory effects of spin glasses, the disorder induced conductor-to-insulator transition in electronic or bosonic systems, the collective behavior of magnetic flux lines in amorphous high temperature superconductors, and the roughening transition of a disordered charge density wave systems are only a few examples for these fascinating phenomena that occur due to the presence of quenched disorder.

Analytic studies of models for these systems are usually based on perturbation theories valid for weak disorder, on phenomenological scaling pictures or on mean-field approximations. Therefore the demand for efficient numerical techniques that allow the investigation of the model Hamiltonians of disordered systems has always been high. Three facts make life difficult here: 1) The

regime, where disorder effects are most clearly seen, are at low temperatures – and are even best visible at zero temperature; 2) the presence of disorder slows the dynamics of theses systems down, they become *glassy*, such that for instance conventional Monte-Carlo or molecular dynamics simulations encounter enormous equilibration problems; 3) any numerical computation of disordered systems has to incorporate an extensive disorder average.

In recent years more and more model systems with quenched disorder were found that can be investigated numerically 1) at zero temperature, 2) without equilibration problems, 3) extremely fast, in polynomial time (for a review on these developments see [1,2] and [3] for an introduction to the non-expert). This *is* indeed progress, which became possible by the application of *exact* combinatorial optimization algorithms developed by mathematicians and computer scientists over the last few decades. This gift is not for free: first a mapping of the problem of finding the *exact* ground state of the model Hamiltonian under consideration onto a standard combinatorial optimization problem has to be found. If one is lucky, this problem falls into the class of P-problems, for which polynomial algorithms exist. If not, the intellectual challenge for the theoretical physicist remains to reformulate the model Hamiltonian in such a way that its universality class is not changed but a mapping on a P-problem becomes feasible. In this paper we review some of the recent progress that has been made in this direction.

2 Elastic manifolds

A system of strongly interaction (classical) particles or other objects, like magnetic flux lines in a type-II superconductor, or a charge density wave system in a solid, will order at low temperatures into a regular arrangement a lattice (crystal lattice or flux line lattice). Fluctuations either induced by thermal noise (temperature) or by disorder (impurities, pinning centers) induce deviations of the individual particles from their equilibrium positions, see Fig. 1. As long as these fluctuations are not too strong an expansion of the potential energy around these equilibrium configuration might be appropriate. An expansion up to 2nd order is called the elastic description or elastic approximation, which in a coarse grained form (where the individual particles that undergo displacements from their equilibrium positions do not occur any more and are replaced by a continuum) reads then

$$H_{\rm elast.} = \int d\mathbf{r} (\nabla u)^2 \quad \stackrel{\rm lattice}{\longrightarrow} \quad \sum_{\langle ij \rangle} [u(r_i) - u(r_j)]^2 \ , \tag{1}$$

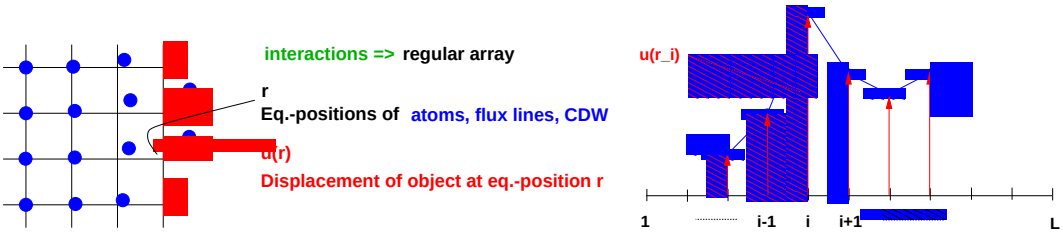

Fig. 1. **Left:** Sketch of a crystal lattice of particle that is slightly distorted by fluctuations. **Right:** A one-dimensional example, which is equivalent to a directed polymer in a random $2d$ environment or the KPZ equation in $1{+}1d$.

where $u(\mathbf{r})$ is the displacement field. The right part of this equation is the lattice version of the continuum description on the left, which is most conveniently studied in numerical approaches.

The effect of impurities, i.e. frozen in or quenched disorder, is described by a random potential

$$H_{\text{rand.}} = \int d\mathbf{r} V[\mathbf{r}, u(\mathbf{r})] \; . \tag{2}$$

Usually one takes V to be a Gaussian, uncorrelated random variable. The lattice version of the resulting Hamiltonian

$$H = \sum_{\langle ij \rangle} (u_i - u_j)^2 + \sum_i V_i(u_i) \tag{3}$$

and the resulting configuration space for the $1d$ case is shown in Fig. 1 (this case is actually in the same universality class as the Kardar-Parisi-Zhang (KPZ) equation describing surface growth).

At low temperatures the physics of the systems described by Hamiltonian (3) is dominated by the disorder so that their universal geometrical properties can directly be studied at zero temperature. At $T = 0$ the elastic manifold in a random environment (3) is in the state of lowest energy and its universal properties can be deduced by studying the average transverse fluctuations in the ground state, the roughness: $w^2 = \sum_i (u_i - \overline{u})^2 \propto L^\zeta$. The universal roughness exponent is $\zeta = 2/3$ in $d = 1$ (exact) and $\zeta = 0.41$ in $d = 2$ and $\zeta = 0.22$ in $d = 3$ (numerical, [4]).

How to solve the problem of finding the exact minimum energy configuration of (3)? The displacement configuration $\{u\}$ forms actually an interface in $d{+}1$ dimension and one can therefore map (3) onto an interface Hamiltonian for a random bond Ising ferromagnet (RBIM) with anti-periodic boundary conditions (see Fig. 2). For this problem one can apply the minimum-cut/maximum-flow algorithm from combinatorial optimization which has a polynomial complexity and is therefore superior to any stochastic method like Monte-Carlo

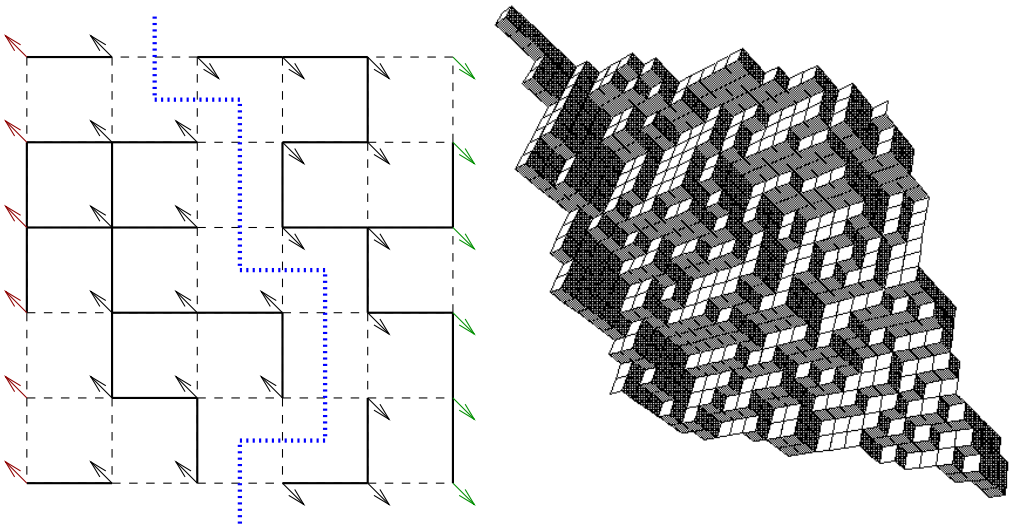

Fig. 2. **Left:** Sketch of a $2d$ (RBIM) with anti-periodic boundary conditions. Broken lines represent weak bonds, full lines strong bonds, the spin configuration with lowest energy defines an interface, as indicated, and corresponds to the minimum cut in the corresponding network flow problem. **Right:** An optimal interface in the 111-direction of a $3d$ RBIM corresponding to the ground state configuration of a $2d$ elastic media with scalar displacement field (from [4]).

or simulated annealing. The aforementioned exponents are then estimated by performing a finite size scaling analysis of roughness data averaged over typically 10^4 different disorder configurations.

3 Periodic elastic media

Flux line arrays like the Abrikosov flux line lattice or charge density wave systems have an important symmetry: The Hamiltonian has, for instance, to be invariant under a global shift of the displacement field by multiples of the lattice constant (see Fig. 3), since this gives, up to boundary term which can be neglected in the infinite systems size limit, the same flux line configuration: $H\{u\} = H\{u + a\}$. The elastic energy (1) definitely has this symmetry, but the random potential V_{random} in (2) has to be modified. Keeping only the first harmonics the most commonly studied case is (one can show that higher harmonics are indeed irrelevant in the RG sense)

$$V[\mathbf{r}, u(\mathbf{r})] = \cos[2\pi\, u(\mathbf{r})/a - \theta(\mathbf{r})], \quad \theta(\mathbf{r}) \in [0, 2\pi] \quad \textbf{random}. \tag{4}$$

The complete lattice Hamiltonian then reads

$$\Rightarrow H = \int d\mathbf{r}\{(\nabla u)^2 + \lambda \cos[2\pi\, u(\mathbf{r}) - \theta(\mathbf{r})]\} \tag{5}$$

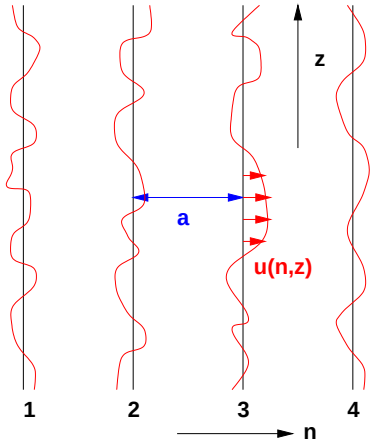

Fig. 3. A $2d$ flux line array. The straight vertical lines indicate the equilibrium position of the individual flux lines without fluctuations.

A naive Flory argument yields for the mean transverse fluctuations (at $T = 0$) $\langle u^2 \rangle \propto \ln(L/L_\xi)$ in $d \leq 4$, but in $2d$ more accurate functional renormalization group calculations yield $\langle u^2 \rangle \propto \ln^2(L/L_\xi)$, where L_ξ is the Larkin length.

Again the ground state of the Hamiltonian (5) can computed in polynomial time by realizing that the $T = 0$ configuration of displacement field corresponds to the optimal interface in a RBIM, but now with *periodic* disorder due to the symmetry requirement (4), which is then again a Min-cut/max-flow problem [5]. Alternatively in $2d$ the interface problem is also equivalent to a solid-on-solid model on a disordered substrate, which amounts to a minimum-cost-flow-problem (also solvable in polynomial time [6]) or to a dimer covering model on a hexagonal lattice with random weights, which amounts to a minimum weighted matching problem [7]. The aforementioned predictions, i.e. logarithmic roughness in $3d$ and log-square roughness in $2d$, have been confirmed with extensive studies using these mappings and algorithms.

A further enrichment of the physics in these elastic media is provided by the presence of a periodic potential, like a lattice potential, whose periodicity, say p, is commensurate with the periodicity a of the elastic medium. The periodic potential favors the flat state ($u = 0$) of the elastic medium whereas the random potential tries to push it into a rough state. These competition of pinning forces leads to roughening transition for strong enough disorder in dimensions $d > 2$ [8]. This new phase transition can be investigated via ground state calculations by incorporating the periodic potential into the Hamiltonian for an elastic medium:

$$H = \int d^d\mathbf{r} \left[\frac{\gamma}{2} |\nabla u|^2 - v \cos(pu) + \eta \cos(u - \theta) \right] \tag{6}$$

On a coarse-grained level, the medium can be described by an integer height variable $\{h_\mathbf{x}\}$ representing a $(3+1)$-dimensional surface on a simple cubic

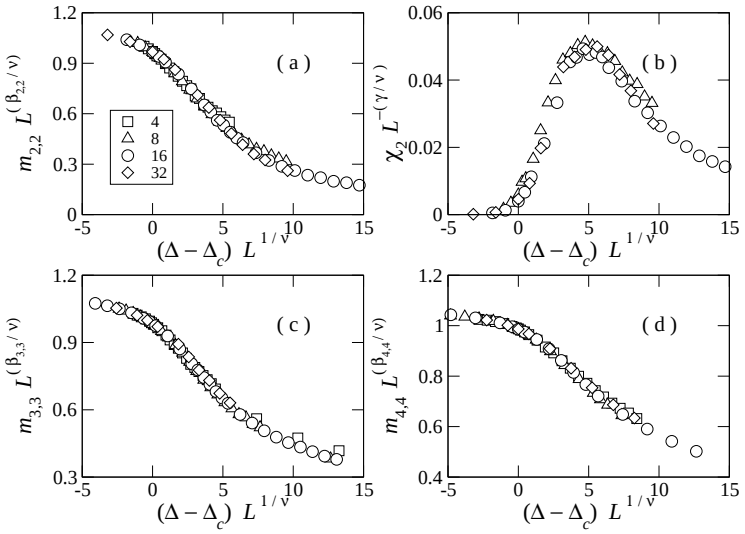

Fig. 4. Scaling plots of the magnetization for $p = 2$ (a), $p = 3$ (c), $p = 4$ (d), and the susceptibility for $p = 2$ with $\gamma/\nu = 2.90$ (b). Parameters used in the plots are mentioned in the text.

lattice with sites $\mathbf{x} \in \{1, \ldots, L\}^3$. Creating steps costs elastic energy and the surface is subjected to a random pinning potential. These effects plus the periodic potential are incorporated in the following solid-on-solid (SOS) model Hamiltonian

$$H = \sum_{(\mathbf{x},\mathbf{y})} J_{(h_\mathbf{x},\mathbf{x});(h_\mathbf{y},\mathbf{y})} |h_\mathbf{x} - h_\mathbf{y}| - \sum_\mathbf{x} \eta_\mathbf{x} \cos[(2\pi/p) h_\mathbf{x} - \varphi_\mathbf{x}] \ , \tag{7}$$

where the first sum runs over nearest neighbor pairs $(\mathbf{x}, \mathbf{y})$ on a simple cubic lattice. The Hamiltonian has to be be invariant under a global shift $h \to h+p$, which is inherited from the symmetry under $\phi \to \phi + 2\pi$ of the continuum Hamiltonian (6). Hence one imposes a periodicity in the step energies J by $J_{(h+p,\mathbf{x});(h'+p,\mathbf{y})} = J_{(h,\mathbf{x});(h',\mathbf{y})}$. Convenient choices for the disorder are a uniform distribution for $0 \le \varphi_\mathbf{x} < 2\pi$ and $0 \le \eta_\mathbf{x} < V$ and an exponential distribution, $P(J) = J_0^{-1} e^{-J/J_0}$, for $J > 0$. The ground state of this Hamiltonian finds again its analogue in an optimal interface in a $4d$ RBIM with the appropriate bond strengths taken from (7).

The numerical study of the $2d$ case [9] shows indeed that the interface, and therefore the elastic medium is always asymptotically rough, independent of disorder strength and periodicity. In $3d$ a roughening transition appears at a critical ratio $\Delta \equiv V/J_0$ [10]. The order parameter is $m_p(L, \Delta) = \langle |e^{2\pi i h_\mathbf{x}}| \rangle$ and the corresponding susceptibility $\chi_p = L^3(\langle |e^{2\pi i h_\mathbf{x}/p}|^2 \rangle - \langle |e^{2\pi i h_\mathbf{x}/p}| \rangle^2)$. A thorough finite size scaling analysis [10] yields the critical exponents $\nu \approx 1.3$ (correlation length exponent), $\beta \approx 0.05$ (order parameter exponent), and $\gamma/\nu \approx 2.9$ (susceptibility exponent), see Fig. 4, which deviate significantly from the functional renormalization group predictions [8].

4 Conclusion

We have shown how ground state calculations can reveal a lot of the physics contained in elastic glass models at zero temperature. In this context an intriguing question is: in how far is the elastic approximation justified? Would topological defects like dislocations occurring in the physical system at hand but *not* contained in the elastic description actually proliferate and destroy the elastic glass phase? In $2d$ this question has been answered in the affirmative [11], but a numerical study in $3d$ of this important, if not crucial question, is still lacking. We hope to have demonstrated that combinatorial optimization methods are an extremely valuable tool in studying the statistical physics of disordered systems — exemplified by the field of elastic glass models.

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