VARIATIONAL PROBLEMS OF INTERACTING DISORDERED PHYSICAL SYSTEMS

1. Introduction

Strongly interacting physical systems, in the presence of disorder, lie at the foundation of the new, nowadays ubiquitous, micro-technologies. In particular, systems of interacting electrons, moving in disordered electromagnetic fields (such as Quantum Hall systems, Anderson-Mott insulators, etc) [1, 2], or mesoscopic samples of carbon nanotubes, etc. are quickly becoming the focus of applied physical and technological efforts.

At this moment, a significant number of well formulated open theoretical problems related to these systems cannot be approached with the standard methods of theoretical physics. In a few words, the recurring question encountered here is the following: a paradigm of theoretical physics is that the equilibrium configuration, or macroscopic state, or ground state (depending on the particular theory) can be obtained uniquely by solving a variational problem with a globally convex (scalar) potential. Characteristically, systems of interacting, disordered systems cannot be described by this approach, as we indicate in subsequent sections. Therefore, new ideas and methods from non-linear polynomial optimization and the analysis of free variables are expected to essentially contribute towards solving some of the theoretical problems of interacting disordered physical systems.

To give a single example of a new trend in optimization theory with a high expectation of applicability to such questions we mention the following Striktpositivstellensatz. We denote by $\mathbf{R}[x]$ the algebra of real polynomials in the commuting variables $x = (x_1, ..., x_n)$ and by $\Sigma\mathbf{R}[x]^2$ the convex cone of sums of squares of polynomials. Let

$$S = \{x \in \mathbf{R}^n;\ f_1(x) \geq 0, ..., f_n(x) \geq 0\}$$

be a basic semi-algebraic set contained in the unit ball $\|x\| \leq 1$. Let $f_0(x) = 1-|x|^2$. Then the following statement holds (see [3]) :

Assume that a polynomial h satisfies $h(x) > 0$ for all $x \in S$. Then

$$h \in \Sigma\mathbf{R}[x]^2 + f_0\Sigma\mathbf{R}[x]^2 + ... + f_n\Sigma\mathbf{R}[x]^2.$$

Thus, when interested in minimizing a polynomial on the basic semi-algebraic set S, one can relax the condition $h_0 = \min_{x\in S} h(x)$ to $h(x) - h_0$ is a weighted sum of squares, as above. This statement simplifies many global optimization problems, and it is the origin of a variety of novel applications, see for instance the pioneering articles by J.-B. Lasserre [4, 5], P. Parrilo [6] and the survey [7].

The unusually rich overlap of problems and methods, as well as the wide, high level of interest in this class of questions, makes this class of problems particularly relevant for fields such as: (1) non-commutative algebraic geometry and non-commutative probability, and (2) polynomial optimization theory, as well as (3)

"glassy" phase transitions for disordered, interacting physical systems; (4) maximum entropy methods for singularity formation in PDE's; and (5) stochastic processes in high-dimensional spaces and data compression.

2. Variational problems in physical systems: a list of examples

We sketch below a few specific open problems from the physics of strongly interacting and correlated systems, which will substantially benefit from the newly developed methods of polynomial optimization and free probability theory.

2.1. **Free probability analysis for quantum communication channels.** Hybrid communication channels (where encoding and decoding are performed using a quantum algorithm, but the transmission still relies on a classical channel) are quickly occupying a prominent place in practical applications of quantum information theory. The theoretical analysis of such systems relies on a probability theory for non-commutative variables, in particular on the free probability theory developed by D.V. Voiculescu [8].

Of special interest in this context is the general field of *estimation* within free probability. This requires generalization of concepts such as Maximum Likelihood Principle, Minimum Variance Unbiased Estimators, etc., in order to enlarge their area of applicability to random variables from infinite-dimensional spaces. From a mathematical point of view, there are interesting connections with the matrix polynomial optimzation, sum of squares problems, etc.

2.2. **Maximum-entropy methods for classical and quantum systems.** A problem which interpolates between the standard, equilibrium classical inference and the free-probability inference, is finding maximum-entropy criteria for physical systems described by non-operator variables, but otherwise out-of-equilibrium. For example, it is known that the evolution of flows described by Euler equations with conservation laws of hyperbolic type leads to singularity formations [9], such as cusps and shocks. Often, it is possible to continue the solution beyond the singularity, in a properly defined weak sense, but this leads, in turn, to a selection problem. A maximum entropy-creation criterion, such as the Lax-Oleinik principle for the case described here, has been used for several decades. Developing the same kind of criterion for more general problems (singularity formation in constrained conformal map dynamics is just one example [10]) is a problem which presents considerable theoretical and practical interest in several areas of science [11, 12].

2.3. **Constraint satisfaction problems in the limit of many variables.** As indicated in the review [7], methods from real algebraic geometry, positive polynomials with matrix variables, etc. have been rediscovered with much interest by application-driven researchers working in the general area of combinatorial optimization, complexity theory and constraint satisfiability (K-Sat). In a nutshell, K-Sat consists of n variables x_i (which may be Boolean) that are supposed to satisfy $k < n$ constraints $f_k(x_i)$. The constraints may be linear, with arbitrary number of variables, or nonlinear, with a fixed (for example, 3) number of variables.

It is known [2] from numerical experiments that, in the large n, k limit, the percentage of satisfied constraints for the optimal solution depends only on the ratio $\phi = k/n$, and the system seems to undergo the analogue of "phase transitions" as ϕ is increased from 0 to values close to unity. Understanding the details of this behavior is very important both for computer science and physics applications.

2.4. **Jamming: optimal configurations with local and global constraints.** The original, rather simplistic formulation of jamming requires finding the highest-density arrangement of identical objects (for example, spheres in 3 dimensions) within a given domain. The geometric constraints are an example of "hard" (or contact) potentials. In a more general formalism, the inter-particle potentials may be smoother, with power-law decay [13]. Moreover, global topological and geometric constraints [13] make the problem completely non-trivial.

This problem is very relevant because of its connections to topics which range from mathematics (potential theory), to physics (granular flow, turbulence) and even more applied areas (material design, functional networks).

2.5. **The glass transition in 2 and 3 dimensions.** Deeply related to jamming, the glass transition is perhaps the most famous open problem in classical condensed matter theory. A summary introduction [14, 15] could be the following: consider the lattice $\mathbb{Z}^d$ ($d = 2, 3, ...$), and variables $\sigma_i = \pm 1, i \in \Omega \subset \mathbb{Z}^d$. The interaction between these variables (*spins*) is encoded in the matrix of interaction constants $J_{ik}, i, k \in \Omega$, which may be taken to be *finite-band*, $J_{ij} = 0$ if $|i - j| > b$ (fixed constant), and whose non-zero entries are distributed with some prescribed law $P(J)$ implementing the disorder. A random *magnetic field* $h_i, i \in \Omega$ and inverse temperature $\beta > 0$ complete the model, whose possible configurations $\mathcal{S} \in \{-1, 1\}^{\mathrm{card}(\Omega)}$ are prescribed the weights

$$W(\mathcal{S}) = \exp \beta \left[\sum_{i,j \in \Omega} J_{ij} \sigma_i \sigma_j + \sum_{i \in \Omega} \sigma_i h_i \right]_{\sigma_i \in \mathcal{S}} .$$

If the interaction constants may take both positive and negative values with finite probability, then finding the most likely configuration, at fixed magnetic field, is believed to be an NP-complete problem. In particular, the corresponding thermodynamic potential is again non-convex.

2.6. **Metal-insulator transition in two dimensions.** Metal-insulator transition (MIT) may be regarded as the quantum version of the glass transition. The fact that a system of electrons may "freeze", i.e. behave like an insulator, because of either strong interactions (Mott transition) or strong disorder (Anderson transition) has been known for roughly half a century [1]. However, creating a theoretical model which could incorporate both interactions and disorder in a proper fashion, was difficult to achieve. The foundation for our current formulation of this problem was laid by Wegner [16], and later improved by Efetov [17]. A clear exposition of this formalism, based on random matrices and *supersymmetry*, can be found in [18, 19].

The difficulties related to this formulation of the problem are due to the fact that the transition cannot be described within the established models of phase transitions. "Proper" phase transitions are characterized by potentials that are globally convex. However, the supersymmetric formulation of MIT does not lead to a true extremum, but rather a saddle-point, due to the non-compact, hyperbolic geometry structure of the effective theory ($SU(1, 1)$ in the simplest case). A resolution is expected to be obtained from generalized, free probability analysis [20].

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