Statistical mechanics: Models and realities

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Studies of statistically (self-) organized complex systems (or networks) are promising remarkable understanding of the emergence of order in nature. Among other things, the availability of cheap computer power on the scientist's desk-top is responsible for this recent spectacular growth in the statistical mechanical studies of such complex systems. The possibilities of the growth of such studies in the Indian Universities/Institutes are briefly discussed.

Statistical physics is presently in a rapidly expanding state; this includes both statics and dynamics of complex condensed matter systems (e.g. porous media, random aggregates, polymers, complex fluids) and complex dynamical networks (e.g. models for neural networks, immune networks, or even economic networks). The established growth, up to this point of time, has mainly been in classical statistical mechanics. Here, a number of key concepts and ideas have emerged and developed: scaling[1], self-similarity and fractal correlations[2], replica symmetry and its breaking in frustrated systems[3], period doubling and other routes to chaos in nonlinear systems[4], spontaneous organization of irreversible dissipative systems (synergetics[5] and self-organized criticality[6]), etc. These concepts have found wide and very appropriate applications in other areas of physics/science: e.g. scaling in quantum statistical physics[7], scaling and the concepts of replica symmetry breaking in the biophysics of brain models[8], chaos and self-organized criticality in earthquake size-distributions and in various economic phenomena[6,9].

This spectacular growth in statistical mechanics has required the attention of a large community of physicists, mathematicians, engineers, economists, etc. Also, the publication of these results not only inflated the sizes or the volumes of the existing (exclusively statistical mechanics) journals (like *Physica* A, *J. Stat. Phys.*, etc.), but also required separate publication of statistical mechanics sections of several established journals (e.g. the *Phys. Rev. E* started out separately from the last year, and is already competing in size with its parents *Phys. Rev. A & B*). Besides, many new journals (e.g. on fractals, nonlinearity, neural networks, etc.) have appeared within the last five years or so to accommodate the research literature in this field. In fact, it is said that we are 'witnessing the creation of new Sciences of Complexity', out of the investigations in complex condensed matter systems (like spin glasses, etc.), and that these new sciences 'may well occupy the center of intellectual life in the twenty-first century'[10].

The emergence of these new sciences of statistical mechanics of complex systems, has in part been due to the new questions and the development of new ideas, mainly in the context of random condensed matter systems (critical phenomena in magnetic systems, random aggregates like DLAs, percolating systems, spin glasses, etc.) and in some cooperative dynamically organized systems (critical dynamics in some nonlinear cellular automata and frustrated magnetic systems). Together with these ideas, the advent of computer graphics, etc., and the availability of undreamed-of computer power on the scientist's desktop, have almost brought about the birth of these new sciences.

Models of complex condensed matter systems

A large amount of recent efforts have been to develop appropriate models of random materials, like the glasses, porous media, quasi- and liquid crystals, polymers, and other complex fluids, which constitute a large part of our natural environment as well as a substantial part of synthetic and artificially produced materials. Many of the lattice models, like the self-avoiding walk models for studying the linear polymer conformational statistics[11], percolation models for studying the physical properties (including breakdown/fracture) of porous media and random composites[12], spin glass models of randomly frustrated magnets[3] and the ANNNI models of various commensurate and incommensurate structures in magnets, crystals, etc.[13], are now established to be very accurate. The ready possibility of (Monte Carlo) simulation of such systems (with discrete interacting degrees of freedom)[14] for realistic sizes (of the order of Avogadro number of degrees of freedom, as in the case of pure Ising system where sizes have gone up[15] to 10^{20}) on computer, allowed very careful checks of the possible theoretical ideas and established the successful models and ideas in a fairly quick and robust way. Size limitation (presently of the order of 10^2–10^3) for the molecular dynamic simulations of classical fluids (with continuous degrees of freedom) or solids, is still the bottleneck for realistic comparisons of the model results.

Our understanding of the condensed quantum matter (magnets, interacting fermion or boson aggregates, etc.) have also been improved in recent years, with the emergence of many new ideas (e g. the proposed spin liquid ground state of frustrated quantum magnets) and with the attempts to check these possibilities in the ground state of the numerically diagonalized finite systems, or using the quantum Monte Carlo methods[16]. However, the difficulties of diagonalizing large matrices and the time (Trotter)-dimension anisotropy of the quantum Monte Carlo methods, forbid simulations of reasonable sizes of quantum systems (presently of the order of $2–3 \times 10^1$ for exact diagonalization and 10^2 for quantum Monte Carlo). In fact, this limitation of the realistic comparison of the model results for quantum condensed matter, has been partly responsible for a rather slow progress in developing and establishing the valid ideas for such systems (compared to classical condensed matter systems).

Reality and prospect

No doubt, many of the models of classical random condensed matter systems are now quite matured and realistic. In many of these cases the crucial ideas and concepts were first established by comparing and checking with the computer simulation results of the models, rather than comparing them with the real experimental results, which were often influenced by other (uncontrollable) physical effects not under study and, in that sense, less accurate compared to the model simulation results. Many of the dynamical (cellular automata) models of frustrated networks are appearing to be very promising, in the sense that they are able to capture some of the essential emerging features of very commonly encountered random, nonlinear and competing network systems: like the associative memory function of the brain in the Hopfield model[8], the self-organized criticality of the earthquakes[6], instabilities and chaos away from the Walrasian equilibrium in economic systems, in the Samuelson's dynamical model (Zhang[9]), etc.

As mentioned before, the prospect of these studies of statistical properties of condensed matter systems (random and complex materials, composites, etc.) and of complex frustrated networks (like neural networks, economic networks, etc.) are enormous. Indeed, these studies seem to promise a major scientific attraction for the rest of this century and perhaps the early one or two decades of the next one. Expectations are enormous: Understanding of the new materials, composites, frustrated quantum magnets, high temperature superconductivity, development of adaptive (or genetic) programs, development of artificial networks with associative and inductive capabilities (with of course the speed of the silicon devices) to generalize from partial examples, incomplete time series, etc., are some of the immediate and exciting goals.

The Indian scene and recommendations

Unlike some of the brilliant contributions in the recent past in the theory of condensed matter systems, like the problem of ground state of low dimensional quantum antiferromagnets, freezing of simple liquids, etc., we have not made any mark yet in developing any realistic modelling in any area of complex systems. Although, very recently there has been some growth in interest as well as in the size of the available manpower etc., the overall encouragement and the efforts are not yet optimal for assuring any meaningful contribution. Apart from a question of attitude (in taking the trouble, and also the pleasure, of comparing, checking and rejecting/establishing our theoretical ideas with our own 'computer experiment' results), the problem lies in a quick and accurate disbursement of these exciting research problems and results to the young graduate/research students (in the Universities).

In the early days of nuclear physics, when the excitement and the potential was established, special teaching/training programme started in various research centres (e.g., in Saha Institute of Nuclear Physics, Bhabha Atomic Research Centre, Tata Institute of Fundamental Research, etc.) Quickly, with their help, and also with the help of their students, various Universities started introducing special courses (papers) in the University teaching (M Sc Physics) programme. This motivated a large number of young researchers who, subsequently with their contributions, made the programme robust and successful. However, studies in nuclear sciences required a substantial investment (which unfortunately is still being continued) and this required the initial patronage of some heavily funded centres to begin with.

I personally think, if (and when) the excitement and the prospect of the statistical mechanical studies of the 'sciences of complexity' (including the theories and applications of neural networks, computers, etc.) are firmly established, efforts should be immediately made to evolve a course (see e.g. ref. 8) for its offer and inclusion as a special paper in M Sc Physics (separately perhaps from condensed matter physics, although many of the course materials would be common). This would require comparatively little investment: preferably one computing-workstation (costing about 6 lakhs presently) per teacher and/or 5–6 students; and some yearly grant (of the order of Rs 1 lakh) for procuring books/monographs and for maintainance etc. Of course, before the implementation of the training programme in the Universities, the programme may further be evolved through a series of Summer Schools, Workshops, etc., and started in some of the leading Research Centres/Institutes/Universities of the country (where manpower and some of the facilities already exist).

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3. Mezard, M., Parisi, G. and Virasoro, M. A., *Spin Glass Theory and Beyond*, World Scientific, Singapore, 1987.
4. see e.g. Ford, J., in *New Physics* [ref. 1], p. 348, and references therein.
5. see e.g. Nicolis, G., in *New Physics* [ref. 1], p. 348, and references therein.
6. Bak, P. and Tang, C., *Phys. Today*, 1989, **42**, S27.
7. Thouless D. J., in *New Physics* [ref. 1], p. 209.
8. see e.g. Hertz, J., Krogh, A. and Palmer, R., *Introduction to the Theory of Neural Computation*, vol. I, and Weisbuch, G., *Complex Systems Dynamics*, vol. II, in the Lecture Notes Series of Santa Fe Institute Studies in the Sciences of Complexity, Addison–Wesley, California, 1991.
9. see e.g. Anderson, P. W. *et al.* (eds.), *The Economy as an Evolving Complex System*, Proc. vol. no. V, in the Santa Fe Institute Studies in the Sciences of Complexity, Addison–Wesley, CA, 1988; Zhang, W. -B., *Synergetic Economics: Time & Change in Nonlinear Economics*, vol. 53 in the Springer Series in Synergetics, Springer-Verlag, Berlin, 1991; Glance, N. S. and Huberman, B. A., *Sci. Am.*, 1994, **270**, 76.
10. Simmons, L. M., in *the Series Foreword of the Santa Fe Institute Studies in the Sciences of Complexity* [refs. 8, 9].
11. de Gennes, P. G., *Scaling Concepts in Polymer Physics*, Cornell Univ. Press, Ithaca, 1979.
12. see e.g. the series *Random Materials & Processes* (eds. Stanley, H. E. and Guyon, E.), North Holland, in particular, *Statistical Models of Fracture of Disordered Media* (eds. Herrmann, H. J. and Roux, S.), 1990; Bergmann, D. J. and Stroud, D., in *Solid State Physics* (eds. Ehrenreich, H. and Turnbull, D.), Academic Press, NY, 1992, vol. 46, p. 147.
13. see Yeomans, in *Solid State Physics* (eds. Ehrenreich, H. and Turnbull, D.), Academic Press, NY, 1987, vol. 41.
14. see e.g. Binder, K. (ed.), *Application of Monte Carlo Method in Statistical Physics*, Springer-Verlag, Berlin, 1987.
15. Stauffer D., 1993 (private communication)
16. see e.g. Dagotto, E, *Int. J. Mod. Phys.*, 1991, **B5**, 907; Suzuki M. (ed.), *Quantum Monte Carlo Methods*, Springer-Verlag, Berlin, 1986.

Optoelectronics

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The challenge of the new technology of optoelectronics and photonics is examined briefly, emphasizing the role of research and development cycle in condensed matter science. Some suggestions to improve our inadequate effort in this field in India are also discussed.

A discussion on the topic 'Optoelectronics' is particularly appropriate here, because this [Physics] department started its activities with the excellent tradition of doing optics and condensed matter physics at the frontiers of knowledge, and this institute [IISc] is an ideal place for developing future technologies. The study of optical properties of condensed matter indeed forms the main basis for the technology of optoelectronics. Here I examine briefly in a very general way a few important points related to (i) experimental research in condensed matter science and the development cycle for a new technology, (ii) the challenge of photonics and optoelectronics, (iii) the inadequate Indian effort in optics, semiconductor science and optoelectronics, and (iv) the question whether it is possible to change this situation.

The research and development cycle

In condensed matter research, one is concerned with the exploration of diverse physical phenomena occurring in different kinds of materials. One is interested in knowing properties of these materials, whether exotic or otherwise, in response to a variety of external stimulus and physical conditions. Having gained this basic knowledge and understanding one then tries to modify known systems to design new deliberately structured materials with desired and controlled properties (Figure 1). Doped semiconductors and other solids, superconducting layered systems, semiconductor quantum heterostructures, metallic magnetic superlattices, and other types of nanostructure materials are just a few familiar examples of such deliberately designed materials. Such materials with controlled properties are important because they can be used directly to fabricate real devices for particular technological appplications. In turn, successful fabrication of high-technology devices motivates experimental researchers to study and design new materials with higher levels of complexity and precision. The emergence of optoelectronics technology is the most recent important example of this research and development cycle beyond the existing technology of semiconductor microelectronics.

The challenge of photonics and optoelectronics

The basic philosophy behind the new technology is to develop and fabricate photonic devices in which optical photons (light waves) instead of electronic charge-carriers