Report on the Hausdorff Trimester Program

Mathematical challenges of materials science and condensed matter physics: From quantum mechanics through statistical mechanics to nonlinear pde

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Topics

The last ten to fifteen years have seen a fascinating growth of possibilities to probe matter on the scale of single atoms, both experimentally and by numerical simulation. This has raised hopes for the systematic bottom-up design of materials with largely improved or completely new properties. Material behavior is, however, by no means determined by the properties at the atomic scale alone. Indeed, it is often the collective behavior of a huge amount of atoms, e.g. in the motion and pinning of dislocations, which crucially determines key material features like brittleness, formability and strength. Between the atomic scale and the macroscopic scale there are a large number of scales on which important features including lattice imperfections, precipitates, grains and phase domains arise. An at least equally challenging separation of scales arises in the time domain, from the femtosecond scale of elementary processes to life time analysis of engineering devices on the scale of decades. Thus so called multiscale modelling has become a very common term in materials science and engineering. To go beyond an ad-hoc coupling of phenomenological models is, however, a major unsolved problem and poses fundamental questions for mathematics and theoretical physics.

The aim of this Hausdorff Trimester Program was to bring together researchers with a broad mathematical and scientific background to identify prototype problems where mathematics can provide new insight into the passage between different scales of description.

The focus was on the following three subthemes (ordered roughly by increasing length scale):

- Quantum many-body systems and effective models
- Statistical mechanics of solids and metastability
- Multiscales at the continuum level and material properties

which are described in more detail below.

Goals

Quantum many-body systems and effective models

On a microscopic level, condensed-matter systems are quantum many-body systems. Due to the difficulty of the many-body problem, an efficient mathematical description often starts from so-called effective models, which are formulated in terms of the degrees of freedom that are most directly related to observed phenomena. One goal of the programme was to focus on essential open questions in this area, as for example (i) the proof of existence of equilibrium Fermi liquids in three dimensions, and an analysis of their properties; (ii) control over real-time many-body Green functions, with the aim of a mathematical theory of quantum transport; (iii) a proof of continuous symmetry breaking (e.g. by superconductivity or magnetism) which has not been possible up to now due to the lack of reflection positivity of such models.

In simulation practice one of the most commonly used method is density functional theory (DFT). DFT replaces a quadratic many-body Hamiltonian by a nonquadratic effective single particle problem, replacing a linear PDE on $\mathbb{R}^{3N}$ by a nonlinear PDE in $\mathbb{R}^3$. In principle there is an exact DFT functional that yields the correct ground state single-particle electron density (one minimizes first over all the other degrees of freedom given the single-particle electron density). However, there is no effective way known to derive an explicit expression for this abstract functional. A major open problem is how to obtain DFT (or some variant of it including matrix DFT) as any form of limit or rigorous simplification of many-body quantum mechanics. One key difficulty is that there is no obvious small parameter in the problem.

Statistical mechanics of solids and metastability

The statistical mechanics of fluids and gases is relatively far developed. By contrast, rather little is known regarding the statistical mechanics of solids. One fundamental reason is that key properties of solids such as resistance to shear are strictly speaking not equilibrium properties. If one waits infinitely long a crystal cannot really resist shear and will reorder under applied shear stress, e.g. through the motion of dislocations. Thus many properties of solids are really due to metastability, even if they exist on geological time scales. A key challenge is to find the right way to describe such metastability mathematically (e.g. through the imposition of suitable constraints) and to prove rigorous results.

In more mathematical terms one interesting difference arises in the relevant notions of convexity. A classical result in statistical mechanics says that the free energy that arises in the thermodynamic limit should be a convex function of the relevant macroscopic fields. In nonlinear elasticity, however, it is known that a nondegenerate free energy density cannot be convex, since this would be conflict with the invariance under rigid motions. Instead a natural notion is the nonlocal condition of quasiconvexity (which states that for affine boundary conditions the minimizers should be affine). It is an interesting and unsolved open question, if and how a similar notion of convexity arises in the thermodynamic limit of suitable lattice models. A related issue is the validity of the Cauchy-Born rule, a standard heuristic device to relate atomistic and continuum theories which can be seen as a version of quasiconvexity on the atomic scale.

Multiscales at the continuum level and material properties

Microstructures in solids are typically studied starting from continuum models at the mesoscopic scale, often with a non-convex free energy which favours phase separation. In the last twenty years great progress has been made in the mathematical analysis of pattern formation and its macroscopic effects in models for shape-memory materials, ferromagnetic materials, plastic deformation of crystals, and superconductivity. The best results have been achieved for ground states (or minimizing sequences) where powerful methods of the calculus of variations are available (relaxation, Γ-convergence, proof of scaling laws through upper and lower bounds). One challenge is to understand the influence of stochastic heterogeneities, which have a strong

influence on the dynamics, e.g. through the pinning of phase interfaces. Another challenge is the treatment of lower dimensional structures such as cracks, grain boundaries or dislocations, in particular in dynamics. This raises fundamental questions both in modelling and in analysis. Regarding modelling, an understanding of the basic mechanisms at finer scales will play an important role. Regarding analysis, a major open problem is a consistent description and analysis of the interaction of lower-dimensional singularities. Computationally the direct tracking of lower-dimensional singularities is often inconvenient and one would like to use phase-field models as for example in the Ambrosio-Tortorelli approximation of the Mumford-Shah functional, popular in image analysis and in the modeling of fracture. Their relation to the corresponding sharp interface models, in particular in a dynamical situation, is however not yet understood in detail.

Organization

As in many HIM programmes, the main focus was on informal interaction between programme participants. Due to the strong thematic coupling with activities in the Institute for Applied Mathematics a close collaboration with researchers and visitors at the University of Bonn has been achieved.

Additionally, the following structured activities took place:

Opening Workshop, May 7 - 8, 2012, 5 long talks by scientists from the applied sciences (with mathematicians in the audience) which helped to define, at the beginning of the programme, some important problems in mechanics which may profit from mathematical input.

Minicourse on "A mathematical perspective on the structure of matter", four two-hour lectures by Prof. R. D. James, also organized at the beginning of the programme, which helped set a common language among participants to the programme.

James gave a series of lectures that highlighted the role of discrete groups of isometries in generating some of the most prominent structures emerging in nanotechnology and biology. These groups, matched to discrete structures, were also shown to generate special time-dependent solutions of the equations of molecular dynamics. The solutions make use of the basic invariance of quantum mechanics: frame indifference and permutation invariance. These in turn were shown to have direct analogs for the Boltzmann equation, as well as for the equations of continuum mechanics appropriate to diverse materials. These solutions provide far-from-equilbrium examples of exact solutions of

equations of physics from atomic to continuum scales, and therefore provide key tests for multi scale methods. Numerous open problems were posed, the most prominent being the unexpectedly important role these groups play in rules governing the structure of matter.

Workshop on "Coarse graining and condensed matter physics", June 18 - 20. 15 talks by programme participants and visitors focusing attention to one key topic of the programme, namely, coarse graining.

Happy Hour of Math. Informal lectures held, weather permitting, in the garden and accompanied by small refreshements. Almost 30 talks over the length of the programme, which strongly helped to forster informal interactions among participants. The topics of the talks were spread over the interests of the participants to the programme.

Results

The key result of the programme has been an increased collaboration between the participating scientists, in particular between mathematicians and non mathematicians. Specific results are presented in the publications which resulted from the programme, including in particular the ones listed below. Before listing the individual publications we discuss exemplarily some key results in the three main thematic areas of the programme.

Quantum many-body systems and effective models

One highlight has been work on Bose-Einstein condensates. Bose-Einstein condensates are states of matter having a macroscopic number of particles all described by the same one-particle orbital. When Bose-Einstein condensation takes place, the system exhibits quantum behavior at the macroscopic level. In the last two decades, it became possible to realize and to study Bose-Einstein condensates in labs. In typical experiments one observes the evolution of initially trapped Bose-Einstein condensates at extremely low temperatures.

A nonlinear partial differential equation, known as the Gross-Pitaevskii equation, is often used to describe and predict the evolution of the condensates. From the point of view of mathematical physics, it would be interesting to understand the emergence of the Gross-Pitaevskii equation starting from first-principle many body quantum mechanics.

At the microscopic level, Bose-Einstein condensates can be described as systems of N bosons (particles whose wave function is symmetric with respect to permutations), interacting through a two-body potential with scattering length of order N^{-1} (the scattering length is a physical quantity measuring the effective range of the potential). In this setting, a first rigorous derivation of the Gross-Pitaevskii equation was given by L. Erdős, B. Schlein, and H.-T. Yau in 2010. During the HIM trimester program, a new approach to this problem was developed in [5]. In contrast to all previous results, the new techniques give precise bounds on the rate of the convergence towards the Gross-Pitaevskii dynamics in the limit of large N. Notice that control on the rate of the convergence is very important for applications, where N is large but, of course, finite.

The methods of [5] have been inspired by similar questions concerning many-body quantum evolution in the so called mean field regime, where particles experience a large number of very weak collisions. From the point of view of physics, however, the Gross-Pitaevskii limit is very different and much more subtle than the mean field regime. In particular, it involves strong collisions among the particles, which produce non-trivial correlations. Developing tools to control the resulting correlation structure is one of the main new obstacles faced in [5].

Similar questions can also be asked for the evolution of systems of fermions, described by wave functions which are antisymmetric with respect to permutations. Of course, in this case there is no Bose-Einstein condensation. Instead, in appropriate regimes, the state of the system can be described by a Slater determinant. It turns out that the evolution of an initial Slater determinant can be approximated by the nonlinear Hartree-Fock equation. From the point of view of mathematical physics, it is interesting to provide a rigorous derivation of this equation, starting from first-principle quantum mechanics. For sufficiently regular interactions, such a derivation has been recently obtained in [7, 6], based also on preliminary discussions which took place at HIM during the trimester program. Notice that, compared with the bosonic case, system of fermions have an important additional property, which makes the analysis much more involved: because of the antisymmetry of the wave functions, the mean field regime of fermions case is naturally coupled with a semiclassical limit.

A related problem concerns the study of the time evolution of the Fröhlich polaron, an electron coupled to the quantized excitations of the background lattice, which is used in the physics literature to describe superconductors.

In the strong coupling limit, it turns out that the dynamics of the polaron can be approximated by an effective equation for the electron wave function [22].

Another important result concerns dissipation and transport theory. A derivation of phenomenological dissipative laws for energy and charge transport, such as Ohm's law and Joule's law, starting from quantum mechanics, has been an important open problem in mathematical physics for a long time. In [10], existence and finiteness of the conductivity measure is proven for macroscopic scales. In [11], the heat production of a many-fermion system caused by external electrical fields is defined as Araki's relative entropy for states on the CAR C^* algebra, and the first law of thermodynamics is proven. This also allows to verify Joule's law by giving the rate at which electrical energy is converted to heat energy. The results in [10, 11] is for a system of free fermions, i.e. without a two-body interaction, but the method of proof is expected to carry over to the case of weakly interacting particles.

Statistical mechanics of solids and metastability

One important theme was the study of phenomena of metastability of materials that undergo first-order diffusionless phase transformations. These exhibit hysteresis loops as the temperature is cycled back and forth through transformation. These loops do not collapse to zero as the temperature is cycled more and more slowly, and therefore are theorized not to be linked to dissipative processes arising from viscosity or thermal activation, but rather to metastability (Zhang, James and Müller, Acta Materialia 2009). Mathematically, the current (incomplete) understanding is that this metastability is linked to an energy barrier. During the program, special conditions on the lattice parameters of the two phases were studied that reduce this barrier, summarized in [14].

In experimental work that occurred parallel to the program, a series of alloys were prepared by systematically pursuing these theoretical conditions on lattice parameters. These led to the new alloy $Zn_{45}Au_{30}Cu_{25}$. In tests that took place shortly following the program, this alloy showed record low hysteresis and record high reversibility among alloys with similar big first order phase transformations [31]. The reasons for this are believed to be linked to the special conditions, but a full understanding is currently unknown.

A second highlight in this area is the development of a new version of two-scale convergence in the context of statistical mechanics [27]. The main tool

which was developed during the stay of the authors at HIM is the construction of Young measures on compacts which are themselves equi-tight sets of Radon measures. Also in the deterministic context of Γ-convergence this leads to a stricter notion of convergence of microstructures. In principle this can be also extended to the multiscale case. But in its present form the result produces gradient Gibbs measure valued Young measures from elasticity type lattice Hamiltonians.

The results of [27] also include a large deviation principle which justifies the usual continuum free energy $\int_\Omega W(\nabla u)$ as the rate functional related to the Gibbs measure defined by a microscopic Hamiltonian. It is shown under rather general assumption that W is always quasiconvex. It is of great interest to know at which points W is uniformly quasiconvex. For a scalar model problem at low temperature this is being studied by Adams, Kotecký and Müller using the rigorous renormalization approach, developed by Brydges and coworkers. The HIM programme allowed us to make significant progress [1].

Multiscales at the continuum level and material properties

One important line of research has been the investigation of the role of singularities in continuum mechanics and their relation to more regular microscopic models, in particular in the context of dislocations. At a continuum level, dislocations are topological singularities which can be modeled as divergence-free vectorial measures supported on one-rectifiable sets. The theory of relaxation for variational problems on dislocations was developed in [15]. The connection to discrete dislocation models of the Ariza-Ortiz type was also investigated during the program. The relation between the continuum and atomistic descriptions of deformable crystals was also studied, exploiting an new bond-counting approach which builds upon an interesting connection to number theory [30].

A different type of singularity, supported on planes instead of lines, arises in fracture. During the program a new model for ductile fracture was developed, building upon regularized plastic deformation models with sublinear growth which allow for cavitation [16]. The resulting scaling laws have been shown to be in good agreement with experimental measurements of fracture toughness in a variety of materials [17]. Plastic deformation in crystals is generated by slip along slip planes, which also correspond to singularities of the deformation. The relation between the decomposition of the defor-

mation gradient into a regular and a singular part at the microscopic level, and between an elastic and a plastic part at a macroscopic level, was discussed in [29]. A different approach to elastoplasticity, based on the rate-independent large-strain Cosserat theory, was also addressed. In particular, explicit solutions of a two-dimensional shear problem have been obtained, with the micro-rotations being stationary solutions of an Allen-Cahn equation [8]. This leads to the prediction of spontaneous patterning, a possible mechanism for the formation of grains and subgrains in deformed solids. The Allen-Cahn system with inclusions, and in particular incorporating the elastic energy of the precipitates, was studied in [9].

Publications

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