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Mini-Workshop: Multiscale and Variational Methods in Material Science and Quantum Theory of Solids

Organised by
Isabelle Catto (Paris)
Isaac Chenchiah (Bristol)
Ivan Veselić (Chemnitz)
Johannes Zimmer (Bath)

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Abstract. This workshop brought together 18 scientists from three different mathematical communities: (i) random Schrödinger operators, (ii) quantum mechanics of interacting atoms, and (iii) mathematical materials science. Several underlying themes were identified and addressed: variational principles, homogenisation techniques, thermodynamic limits, spectral theory, and dynamic and stochastic aspects.

Mathematics Subject Classification (2000): 35, 49, 70, 74, 82.

Introduction by the Organisers

This workshop brought together people working in probability theory, multiscale analysis, calculus of variations and spectral theory. The purpose was to stimulate exchanges between the respective communities, and identify open problems at the boundaries and intersections of these areas.

There are several mathematical links between the theory of random Schrödinger operators, quantum mechanics of interacting atoms, and mathematical materials science. For instance, spectral analysis lies at the heart of the study of random Schrödinger operators; it is used in the quantum mechanics of interacting atoms as a natural and important tool for the analysis of Euler-Lagrange equations and their solutions; it was shown in the workshop that spectral analysis plays an important rôle in the study of photonic crystal fibres, e.g., in the study of band gaps.

Other tools of scale-bridging were discussed including homogenisation and the computation of the thermodynamic limits of various classical and quantum systems.

Several expository morning lectures explained the fundaments of these fields to the varied audience, particularly to those in the other communities. These lectures were intended to last 60 – 75 minutes but almost always lasted 90 minutes due to lively discussions, both during and after the talks. They were complemented by specialised talks in the afternoon.

The organisers feel that this attempt to bring these different communities together was largely successful, and may have built new bridges between analysis and probability; the credit for this belonging, for the most part, to the speakers. That mini-workshops on "Levy Processes and Related Topics in Modelling" and "Control of Free Boundaries" were being held in parallel afforded many opportunities for further interactions.

There was roughly the same number of analysts and probabilitists among the participants. France, Germany, the UK and the US were about equally represented; there was one participant from Denmark. Almost all participants were relatively early in their careers.

The excellent living and working conditions provided by the institute contributed to a lively scientific atmosphere. The organisers thank the NSF for funding the participation of the three speakers from the US, Patrick Dondl for collecting the extended abstracts (and the "kleine Trommler" for livening up the excursion!).

Mini-Workshop: Multiscale and Variational Methods in Material Science and Quantum Theory of Solids

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Abstracts

The universality classes in the parabolic Anderson model

Wolfgang König

The *parabolic Anderson model* is the Cauchy problem for the heat equation with i.i.d. random potential, i.e.,

$$\partial_t u(t,z) = \Delta^{\mathrm{d}} u(t,z) = \xi(z) u(t,z), \qquad t \in (0,\infty), z \in \mathbb{Z}^d,$$

with initial condition $u(0,\cdot) = \delta_0(\cdot)$. Here $\Delta^{\mathrm{d}} f(z) = \sum_{y\sim z}(f(y) - f(z))$ is the discrete Laplacian, and $\xi = (\xi(z))_{z\in\mathbb{Z}^d}$ is a random i.i.d. potential with values in $[-\infty,\infty)$. The solution $u(t,\cdot)$ is a time-dependent random field. Its almost sure existence is guaranteed under a mild moment condition on $\xi(0)$. The solution $u(t,\cdot)$ describes a random mass flow through a random potential of sinks (sites z with $\xi(z) < 0$) and sources (sites z with $\xi(z) > 0$). The Laplacian has a smoothing effect, while the random potential, the disorder, has the effect of making the solution highly irregular. The parabolic Anderson model is one of the fundamental models for a random motion in a random medium. In terms of the well-known *Feynman-Kac formula*, the solution may be written as

$$u(t,z) = \mathbb{E}_0\Big[\exp\Big\{\int_0^t \xi(X_s)\,\mathrm{d}s\Big\} 1_{X_t=z}\Big],$$

where $(X_s)_{s\geq 0}$ is a continuous-time simple random walk with generator Δ^{d} in $\mathbb{Z}^d$ starting from z under $\mathbb{E}_z$.

We are interested in the long-time behavior of the random field $u(t,\cdot)$. In particular, we want to understand where the main bulk of the total mass,

$$U(t) = \sum_{z\in\mathbb{Z}^d} u(t,z),$$

comes from. Much work is devoted to a thorough understanding of the effect of *intermittency*, which states that, asymptotically as $t\to\infty$, the main contribution to $U(t)$ comes from a few small islands, called the *relevant islands*, which are far away from each other. If all positive exponential moments of $\xi(0)$ are finite, then all moments of $U(t)$ are finite. In this case, intermittency can be defined by the requirement that

$$0 < p < q \qquad \Longrightarrow \qquad \lim_{t\to\infty} \frac{\langle U(t)^p\rangle^{1/p}}{\langle U(t)^q\rangle^{1/q}} = 0,$$

where we write $\langle\cdot\rangle$ for expectation with respect to the potential. (See [3] for an explanation why this corresponds to the above intuitive definition of intermittency.) If $\xi(0)$ is not almost surely constant, then intermittency holds in this sense [3].

However, we want to analyse the behavior of $u(t,\cdot)$ in much greater detail. In particular, we have the following questions:

(1) How large are the relevant islands, and how large are the potential and the solution in these islands?
(2) What do the shapes of the potential and of the solution in these islands look like?
(3) How many relevant islands are there, and what can be said about their distribution in space?

From the above Feynman-Kac formula one sees that the large-t behavior is determined by the upper tails of $\xi(0)$, since $U(t)$ is the t-th exponential moment of $\frac{1}{t}\int_0^t \xi(X_s)\,\mathrm{d}s$. More precisely, we have to find the upper-tail behavior of the principal (i.e., largest) eigenvalue of the operator $\Delta^{\mathrm{d}} + \xi$ in certain large, t-dependent boxes. Hence, the only property of the potential distribution that will enter the description of the long-time behaviour will be the upper tails of $\xi(0)$. We will be working in the case in which all positive moments of $\xi(0)$ are finite.

In [2] it turned out that, under some mild regularity condition on the upper tails of $\xi(0)$, there are precisely four universality classes of asymptotic behaviors of $U(t)$. Let us describe this briefly.

It is convenient to state our assumptions in terms of the logarithmic moment generating function, $H(t) = \log\langle \mathrm{e}^{t\xi(0)}\rangle$. The main regularity assumption is the existence of a continuous scale function $\kappa\colon (0,\infty) \to (0,\infty)$ and of a non-degenerate function $\widehat{H}\colon [0,\infty) \to \mathbb{R}$ such that

$$\lim_{t\to\infty} \frac{H(ty) - yH(t)}{\kappa(t)} = \widehat{H}(y), \qquad y \in [0,\infty).$$

The theory of regular functions tells that $\widehat{H}$ must be either the function $\widehat{H}(y) = \rho y \log y$ for some $\rho > 0$ or $\widehat{H}(y) = \frac{y^\gamma - y}{\gamma - 1}$ with some $\gamma \in \mathbb{R}\setminus\{1\}$. We further assume that $\kappa^* = \lim_{t\to\infty} \kappa(t)/t \in [0,\infty]$ exists. Now we can distinguish the following four classes:

(1) $\gamma > 1$, or $\gamma = 1$ and $\kappa^* = \infty$: This is the so-called double-exponential case with $\rho = \infty$, a degenerate boundary case of the following case.
(2) $\gamma = 1$ and $\kappa^* \in (0,\infty)$: This is the double-exponential case where the upper tails are given by
$$\mathrm{prob}\big(\xi(0) > r\big) \approx \exp\big\{ -\mathrm{e}^{r/\rho}\big\}, \qquad r \to \infty,$$
and we have $H(t) = \rho t \log(\rho t) - \rho t = o(t)$. In this case, [4] analysed the behavior of the moments of $U(t)$ and its almost sure behavior, and [5] proved the geometric picture of intermittency. The relevant islands have a diameter of finite order as $t \to \infty$.
(3) $\gamma = 1$ and $\kappa^* = 0$: This is a new class arising in [2], and the potential is called almost bounded. The moments of $U(t)$ and its almost sure behavior were analysed in [2], and it was phenemonologically found that the potential approaches a perfect parabola in the relevant peaks, and the solution approaches a perfect Gaussian function.

(4) $\gamma < 1$: This is the case of bounded potentials, which was already analysed in [1]. The diameter of the relevant islands grows like a power of t.

In all four classes, the asymptotics of the moments of the total mass can be described in a unifying way by

$$\langle U(t)^p \rangle = \exp\Big\{\alpha(pt)^d H\big(t\alpha(pt)^{-d}\big) - \frac{\chi + o(1)}{\alpha(pt)^2}\Big\}, \qquad t \to \infty,$$

where $\alpha(t)$ is a deterministic scale function defined in terms of $\kappa(t)$, and χ is a characteristic variational formula. Informally, $\alpha(t)$ is the order of the radii of the relevant islands, and the minimizers of χ describe the shape of the potential and of the solution, respectively, in the relevant islands. The formula χ and its minimizers are well understood in the first three classes, but not in the last one. The geometric characterisation of intermittency in the strong sense (i.e., the determination of islands such that the contribution from their complement is negligible) has been proved only in the second class, and in some important special case of the continuous version, the case of Brownian motion among Poisson obstacles [6].

Finding a tight upper bound for the number of relevant islands is an interesting open problem; currently one can bound their number only by a random term of the form $t^{o(1)}$. The centers of the relevant islands should form a Poisson process after rescaling, but this idea has not yet been worked out.

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Singular Limits via the Principle of Maximal Dissipation

Stephen J. Watson

The singular limits of dissipative multi-scale partial differential equations are naturally characterized through the asymptotic expansion of an Onsager-Raleigh-type Principle of Maximal Dissipation ($\mathcal{PMD}$) [1]. We exhibit this schema for solutions $h : \mathbb{R}^2 \times [0, \infty) \to \mathbf{R}$ of the particular evolution equation

$$\frac{\partial h}{\partial t} = \frac{1}{\varepsilon}\mathbf{div}\left[D\widehat{W}\,(\nabla h)\right] - \varepsilon\Delta^2 h, \tag{1}$$

in the limit $\varepsilon \to 0^+$. For simplicity of exposition, we treat the trigonally symmetric potential

$$W(p,q) := -\frac{1}{6}(q^2+p^2) + \frac{1}{9}(q^3 - 3qp^2) + \frac{1}{6}(q^2+p^2)^2\,,$$

which is minimized by the gradients $\nabla h = p\mathbf{i} + q\mathbf{j} \in \mathcal{G}$, where

$$\mathcal{G} := \left\{ \frac{\sqrt{3}}{2}\,\mathbf{i} + \frac{1}{2}\,\mathbf{j}\,, -\frac{\sqrt{3}}{2}\,\mathbf{i} + \frac{1}{2}\,\mathbf{j}\,,\ -\mathbf{j} \right\}.$$

Now, assume that the outer-scale structure of the *solution surface*, $z = h$, is approximated, to leading-order, by the piecewise-affine surface $z = \mathcal{H}$, with $\nabla\mathcal{H} \in \mathcal{G}$. We show that the vertical velocity $\mathcal{V}_i$ of the *ith* facet of $z = \mathcal{H}(\mathbf{x}, t)$ is given by

$$\mathcal{V}_i = -\frac{1}{\mathcal{A}_i}\frac{\partial \mathcal{P}}{\partial \mathcal{H}_i}\,, \tag{2}$$

where $\mathcal{P}$ denotes the (projected) perimeter of the edge-set of $z = \mathcal{H}(\mathbf{x}, t)$, while $\mathcal{H}_i$ is a local height co-ordinate for the *ith* facet. The scaling properties of this Piecewise-Affine Dynamic Surface ($\mathcal{PADS}$) (2) predict the scaling law $\mathcal{L}_\mathcal{M} \sim t^{1/3}$, for the growth in time t of a characteristic morphological length scale $\mathcal{L}_\mathcal{M}$ as the surface coarsens.

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Lifshitz asymptotics for Hamiltonians monotone in the randomness

Ivan Veselić

In various aspects of the spectral analysis of random Schrödinger operators monotonicity with respect to the randomness plays a key role. In particular, both the continuity properties and the low energy behaviour of the *integrated density of states* (IDS) are much better understood if such a monotonicity is present in the model than if not.

In this note we present Lifshitz-type bounds on the IDS for two classes of random potentials. One of them is a slight generalisation of a model for which a Lifshitz bound was derived in a recent joint paper with Werner Kirsch [KV]. The second one is a *breather type potential* which is a sum of characteristic functions of intervals. Although the second model is very simple, it seems that it cannot be treated by the methods of [KV]. The models and the proofs are motivated by well-established methods developed for so called *alloy type potentials*. The basic notions of random Schrödinger operators and the IDS can be inferred e.g. from [CL90, PF92, Sto01, KM, Ves06].

§1 Random Schrödinger operators and the IDS. We consider Schrödinger operators on $L^2(\mathbb{R}^d)$ with a random, $\mathbb{Z}^d$-ergodic potential. More precisely, the random potential $W_\omega \colon \mathbb{R}^d \to \mathbb{R}$ is determined by an i.i.d. family of non-trivial, bounded random variables $\lambda_k \colon \Omega \to [\lambda_-, \lambda_+] =: J$ indexed by $k \in \mathbb{Z}^d$ and distributed according to the measure μ, and a jointly measurable *single site potential* $u \colon J \times \mathbb{R}^d \to \mathbb{R}$. We assume that $\lambda_- \in \operatorname{supp} \mu$ and that $\sup_{\lambda \in J} |u(\lambda, \cdot)| \in \ell^1(L^p)$, $p > \max(2, d/2)$. Under these assumptions the random potential

$$W_\omega(x) = \sum_{k \in \mathbb{Z}^d} u(\lambda_k(\omega), x - k) \tag{1}$$

is relatively bounded with respect to the Laplacian with relative bound zero, uniformly in ω. Consequently, for a bounded $\mathbb{Z}^d$-periodic potential W_{per} the operators $H_{\mathrm{per}} := -\Delta + W_{\mathrm{per}}$ and $H_\omega := H_{\mathrm{per}} + W_\omega$ are selfadjoint on the domain of Δ and lower bounded uniformly in ω. Moreover, $(H_\omega)_\omega$ forms an *ergodic family of operators*. Hence there exist a closed $\Sigma \subset \mathbb{R}$ and an $\Omega' \subset \Omega$ of full measure, such that for all $\omega \in \Omega'$ the spectrum of H_ω coincides with Σ. For $\Lambda_L := [-L/2, L/2]^d, L \in \mathbb{N}$ define the distribution function $N(E) := L^{-d}\, \mathbb{E}\, \{\mathrm{Tr}[\chi_{]-\infty, E]}(H_\omega)\, \chi_{\Lambda_L}]\}$. This function is independent of L and is called IDS or *spectral distribution function*. The support of the associated measure coincides with Σ. The IDS can be approximated in the sense of distribution functions by its finite volume analogs $N_\omega(E) := L^{-d} \sharp\{\text{eigenvalues of } H_\omega^L \leq E\}$ almost surely. Here H_ω^L denotes the restriction of H_ω to Λ_L with Neumann boundary conditions. For many types of random Hamiltonians the IDS is expected to be very "thin" near the spectral minimum $E_0 := \min \Sigma$. More precisely I. M. Lifšic conjectured in [Lif63, Lif64] an asymptotic behaviour of the form $N(E) \sim c e^{-\tilde{c}(E - E_0)^{-d/2}}$ for $E - E_0$ small and positive, where $c, \tilde{c}$ denote some positive constants. The spectrum near E_0 corresponds to very rare configurations of the randomness and E_0 is consequently called a *fluctuation boundary*.

§2 A class of potentials monotone in the randomness. Here we present a slight extension of the main result in [KV]. Assume that the potentials u and W_{per} satisfy the following

Hypothesis A. For any $\lambda \in J$ we have $\operatorname{supp} u(\lambda, \cdot) \subset \Lambda_1$ as well as $u(\lambda, x) \geq u(\lambda_-, x)$ for all $x \in \mathbb{R}^d$. There exist $\epsilon_1, \epsilon_2 > 0$ such that for all $\lambda \in [\lambda_-, \lambda_- + \epsilon_2]$

$$\textstyle\int_{\mathbb{R}^d} dx\, u(\lambda, x) \geq \epsilon_1\, (\lambda - \lambda_-) + \int_{\mathbb{R}^d} dx\, u(\lambda_-, x)$$

and for all $\lambda \in [\lambda_- + \epsilon_2, \lambda_+]$

$$\textstyle\int_{\mathbb{R}^d} dx\, u(\lambda, x) \geq \int_{\mathbb{R}^d} dx\, u(\lambda_- + \epsilon_2, x)$$

hold. The function $\lambda \mapsto u(\lambda, x)$ is Lipschitz continuous at λ_-. More precisely, for some κ, all $x \in \Lambda_1$ and all $\lambda \in [\lambda_-, \lambda_- + \epsilon_2]$ we have $u(\lambda, x) - u(\lambda_-, x) \leq \kappa(\lambda - \lambda_-)$. If $d \geq 2$, then for any $\lambda \in J$ the functions $u(\lambda, \cdot)$ and W_{per} are reflection symmetric with respect to all d coordinate axes

Typical examples of potentials u satisfing Hypothesis A are: an alloy type potential, i.e. $u(\lambda, x) = \lambda f(x)$ with $L^\infty_c(\Lambda_1) \ni f \geq 0$, and a breather type potential, i.e. $u(\lambda, x) = f(x/\lambda)$ with $\operatorname{supp} f \subset \Lambda_{\lambda_-}, \lambda_- > 0, f \in C^1(\mathbb{R}^d \setminus \{0\})$ and $L^\infty(\mathbb{R}^d) \ni g(x) := -x \cdot (\nabla f)(x) \geq 0$.

THEOREM B. (LIFSHITZ BOUND) Under the Hypothesis A the IDS of the Schrödinger operator $H_\omega := -\Delta + W_{\rm per} + W_\omega$ satisfies

$$\lim_{E \searrow E_0} \frac{\log |\log N(E)|}{\log(E - E_0)} \leq -\frac{d}{2} \tag{2}$$

Thus for $E - E_0$ small and positive, asymptotically the bound $0 < N(E) \leq e^{-\tilde{c}(E-E_0)^{-d/2}}$ holds. The proof is essentially the same as in [KV].

§3 Breather potentials with characteristic functions of intervals. We consider a very explicite class of random potentials on $\mathbb{R}$. Let $(\lambda_k)_{k\in\mathbb{Z}}$ be as before with $\lambda_- = 0$, $\lambda_+ = 1$. The breather type potential

$$W_\omega(x) = \textstyle\sum_{k\in\mathbb{Z}} u(\lambda_k(\omega), x - k), \quad \text{where } u(\lambda, x) = \chi_{]0,\lambda]}(x), \tag{3}$$

does not satisfy the Lipschitz condition in Hypothesis A. Nevertheless we have

THEOREM C. The IDS of the Schrödinger operator $H_\omega := -\Delta + W_\omega$, where W_ω is as in (3), satisfies the Lifshitz bound (2). Note that $d = 1$ and $E_0 = 0$ for this model.

It seems that the reason why the method of [KV] is not applicable to the potential (3) is the use of Temple's inequality [Tem28]. For Temple's inequality to yield an efficient estimate, the second moment $\langle H^L_\omega \psi, H^L_\omega \psi\rangle$ in an well chosen state ψ has to be much smaller than the first moment $\langle \psi, H^L_\omega \psi\rangle$. For the current application the best choice of ψ seems to be the periodic, positive ground state of $H_{\rm per}$. However, for such ψ and for the potential (3), the first and second moment coincide! It turns out that Thirring's inequality [Thi94, 3.5.32] is better adapted to the model under consideration. It was used before in [KM83, Mez85] in a similar context.

SKETCH OF PROOF: As before the superscript ^{L} denotes the Neumann b. c. restriction to $[-L/2, L/2]$. Since $N(E) \leq L^{-1}\mathrm{Tr}[\chi_{]-\infty,E]}(-\Delta^L)]\mathbb{P}\{\omega \mid E_1(H^L_\omega) \leq E\}$ for any $L \in \mathbb{N}$, it is sufficient to derive an exponential bound on the probability that the first eigenvalue $E_1(H^L_\omega)$ of H^L_ω does not exceed E.

We set $I_L := \Lambda_L \cap \mathbb{Z}, \alpha := \pi^2, H_0 := -\Delta - \alpha/4L^2$, $\psi = L^{-1/2}\chi_{\Lambda_L}$ and $V_\omega(x) = \alpha/4L^2 + W_\omega(x)$. Then $E_1(H^L_0) = -\alpha/4L^2$ and $E_2(H^L_0) = 3\alpha/4L^2$. Since V_ω does not vanish, V_ω^{-1} is well-defined and we calculate

$$L\left(\int_{\Lambda_L} V_\omega(x)^{-1} dx\right)^{-1} = \frac{\alpha}{4L^2}\frac{4L^2 + \alpha}{4L^2 - 4L^2 S_L + \alpha}.$$

We use the notation $S_L := L^{-1}\sum_{k\in I_L} \lambda_k$ for averages, $\tilde{\lambda}_k := \min(\lambda_k, 1/2)$ for cut-off random variables and similarly $\tilde{V}_\omega$, $\tilde{S}_L$ for cut-off potential and averages.

Then $E_1(H_0^L) + \langle \psi, \tilde{V}_\omega^{-1}\psi\rangle^{-1} \leq \alpha/4L^2 < E_2(H_0^L)$, thus Thirring's inequality is applicable and yields

$$E_1(H_\omega^L) \geq E_1(\tilde{H}_\omega^L) \geq E_1(H_0^L) + \langle \psi, \tilde{V}_\omega^{-1}\psi\rangle^{-1} \geq \tfrac{\alpha \tilde{S}_L}{5L^2}$$

as soon as $L^2 \geq \alpha$. For given $E, \beta > 0$, chose $L := \lfloor \beta E^{-1/2} \rfloor$, then $\mathbb{P}\{E_1(H_\omega^L) \leq E\} \leq \mathbb{P}\{\alpha\tilde{S}_L/5L^2 \leq E\} \leq \mathbb{P}\{\alpha\tilde{S}_L/5 \leq \beta^2\}$. Since $0 < \mathbb{E}\{\tilde{S}_L\} = \mathbb{E}\{\tilde{\lambda}_k\} \leq 1/2$ it is possible to choose $0 < \beta \leq \sqrt{\alpha\,\mathbb{E}\{\tilde{\lambda}_k\}/10}$. With this choice we have $\mathbb{P}\{\tilde{S}_L \leq 5\beta^2/\alpha\} \leq \mathbb{P}\{\tilde{S}_L \leq \mathbb{E}\{\tilde{S}_L\}/2\}$. A large deviation estimate bounds this probability by $e^{-cL} = e^{-\tilde{c}E^{-1/2}}$ for some positive constants $c, \tilde{c}$. This completes the proof.

The higher dimensional analog of this model is currently under study.

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High energy asymptotics for the density of states of unbounded discrete random Schrödinger operators

Frédéric Klopp

The material presented in this talk is taken from [4].

1. Introduction

Let H be a self-adjoint translational invariant Jacobi matrix with exponential off-diagonal decay that is $H = ((h_{k-k'}))_{k,k' \in \mathbb{Z}^d}$ such that, for some $C_0 > 0$ and all $k \in \mathbb{Z}^d$, $|h_k| \leq C_0 e^{-|k|/C_0}$. H defines a bounded self-adjoint operator on $\ell^2(\mathbb{Z}^d)$; it is unitarily equivalent to the multiplication by the function $\theta \mapsto \hat{H}(\theta) = \sum_{k \in \mathbb{Z}^d} h_k e^{ik\theta}$ acting on $L^2([-\pi,\pi]^d)$. The spectrum of H is $\sigma(H) = \hat{H}([-\pi,\pi]^d)$. We define $[\hat{H}_-, \hat{H}_+] = \sigma(H)$.

Consider now the d-dimensional random Jacobi matrix $H_\omega = H + V_\omega$ where V_ω is a diagonal matrix with independent identically distributed real entries denoted by $(\omega_k)_{k \in \mathbb{Z}^d}$ that is

$$V_\omega = \sum_{k \in \mathbb{Z}^d} \omega_k \Pi_k$$

The tail of the probability distribution of the $(\omega_k)_{k \in \mathbb{Z}^d}$ near $+\infty$ will be denoted by $F(\lambda) = \mathbb{P}(\{\omega_0 \geq \lambda\})$. We will assume that the random variables $(\omega_k)_{k \in \mathbb{Z}^d}$ are unbounded from above i.e.

$$F(\lambda) > 0, \quad \forall \lambda \in \mathbb{R}. \tag{1}$$

and that they have a finite expectation

$$\mathbb{E}(|\omega_0|) < +\infty. \tag{2}$$

Moreover we assume that F is absolutely continuous near $+\infty$.

The operator H_ω admits a density of states denoted by $d\nu$ ([2], [9], [1]). $d\nu$ is a positive measure that essentially counts the number of states of the operator per units of volume. It can be defined by

$$\int_{\mathbb{R}} \varphi d\nu = \mathbb{E}\left(\langle \delta_0, \varphi(H_\omega)\delta_0 \rangle\right), \quad \varphi \in \mathcal{C}_0^\infty(\mathbb{R}),$$

where $\mathbb{E}(\cdot)$ denotes the expectation with respect to the random variables $(\omega_k)_{k \in \mathbb{Z}^d}$. Define

$$N(\lambda) = \int_\lambda^{+\infty} d\nu.$$

So, in this talk, N denotes the complementary to 1 of the usual integrated density of states. As simple consequence of the boundedness of H, one has

$$F(\lambda + \|H\|) \leq N(\lambda) \leq F(\lambda - \|H\|). \tag{3}$$

This immediately leads to first order asymptotics for $N(\lambda)$ when F does not decay to fast. Our aim is to present more precise asymptotics for $N(\lambda)$ when λ tends to $+\infty$. As a result, we will be able to study the transition between the classical and

the quantum regime for N i.e between the regime when N is essentially given by F (the classical regime) even at second (or third) order and the regime when the first order correction to the high energy behavior of N really results from tunneling (i.e the quantum regime), the main term still being given by F.

The parameter that will decide whether we are in one regime or the other is the decay rate of F at $+\infty$. This may understood heuristically in the following way. If one interprets N as the probability of H_ω (restricted to some box of size L) having an eigenvalue above level λ, then, this eigenvalue will be created only if, at least one of the random variables $(\omega_k)_k$ is larger than λ. We know that, if we just have a single ω_k that is larger than λ, then, to create an eigenvalue larger than λ, ω_k will have to be larger than $\lambda - h$ where h depends on H and satisfies $h < \hat{H}_+$. The probability of this event will roughly be of size $F(\lambda - h)$. The other extreme option is that sufficiently many ω_k's are larger than $\lambda - \hat{H}_+$. The probability of this to happen is roughly $F(\lambda - \hat{H}_+)^M$ if M is the number of ω_k's larger than $\lambda - \hat{H}_+$. As M is assumed to be large, these two events are essenitally disjoint; so that the probability we want to estimate will be the sum of the two probabilities i.e. it will be the supremum of the two probabilities if one of the probabilities is much larger than the other one. We will be in the classical case if $F(\lambda - h)$ is much larger than $F(\lambda - \hat{H}_+)^M$ and, in the quantum case if $F(\lambda - \hat{H}_+)^M$ is much larger than $F(\lambda - h)$. One convinces oneself that it is the rate of decay of F at $+\infty$ that will determine whether one is the classical or the quantum regime.

2. The results

Define $g = -\ln F$. It is increasing and tends to $+\infty$ at $+\infty$.

2.1. **The classical regime.**

We will say that we are in the classical regime if,

$$\frac{g'(\lambda)}{g(\lambda)} \underset{\lambda \to +\infty}{\to} 0. \tag{4}$$

The precision of our results will then depend on the rate of increase of g and of the precision with which g is known. Under no more assumptions than the one made above, we show the

Theorem 2.1. *Let H_ω and N be defined as above. Then, for any $\delta > 0$, we have*

$$N(\lambda) = F(\lambda + a_0 + o(1)) + o(F(\lambda)^{2-\delta}) \tag{5}$$

where $a_0 = -h_0 = -\dfrac{1}{Vol(\mathbb{T})} \displaystyle\int_{\mathbb{T}} \hat{H}(\theta) d\theta$ is the zeroth Fourier coefficient of $\hat{H}$.

Formula (5) is not very precise but we will see that, under the sole assumption (4), one cannot do better. One can improve on the results of Theorem 2.1 if one assumes a minimal rate of decay for F at infinity. More precisely, if we assume that, for some $\eta > 0$,

$$F(\lambda) = o(\lambda^{-d-\eta})$$

then we get

Theorem 2.2. *Let $f : (0, +\infty) \to (0, +\infty)$ a function tending to 0 at $+\infty$ such that $f(\lambda) \cdot \lambda > 1$.*
Then, there exists $\lambda_\delta > 0$ and $\delta : (\lambda_\delta, +\infty) \to (0, +\infty)$, a positive function such that $\delta(\lambda) \geq f(\lambda)$ and $\lim_{\lambda \to +\infty} \delta(\lambda) = 0$, and such that, for any $\nu > 0$, there exists $\lambda_{s,\nu} > 0$ such that, for $\lambda > \lambda_{s,\nu}$, one has

$$N(\lambda) = F(\lambda + a_0 + a_1/\lambda + \delta(\lambda)/\lambda) \cdot [1 + o(1)] + E_1(\lambda) + E_2(\lambda) \tag{6}$$

where

- *a_0 is defined as in Theorem 2.1 and*

$$a_1 = -\sum_{k \in (\mathbb{Z}^d)^*} |h_k|^2 = \left| \frac{1}{Vol(\mathbb{T})} \int_{\mathbb{T}} \hat{H}(\theta) d\theta \right|^2 - \frac{1}{Vol(\mathbb{T})} \int_{\mathbb{T}} |\hat{H}(\theta)|^2 d\theta,$$

- *$E_1(\lambda) = O(\lambda^{2d} F(\lambda)^{2-\nu})$ and*

$$E_2(\lambda) = O\left(F(\lambda + a_0 + o(1)) F\left(\frac{\delta(\lambda)\lambda}{\ln^d(\lambda/\delta(\lambda))} \right) \ln^d(\lambda/\delta(\lambda)) \right)$$

For $\omega_0 > 0$, consider the operator $H + \omega_0 \Pi_0$. Let $E(\omega_0)$ denote the supremum of its spectrum. Then, for ω_0 large, $E(\omega_0)$ is an eigenvalue of $H + \omega_0 \Pi_0$. It solves

$$\omega_0 \cdot I(E) = 1 \text{ where } I(E) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \frac{1}{E - \hat{H}(\theta)} d\theta.$$

Computing its asymptotic expansion, we see that the principal term in (6) is essentially the probability of $\{E(\omega_0) \geq \lambda\}$. So, the density of states is essentially given by the probability that there is a single eigenvalue larger than λ. In this regime (at this level of precision), the density of states of H_ω does not at all feel the tunneling between the different sites; or it looks like as if one would be dealing with infinitely many i.i.d. copies of $H + \omega_0 \Pi_0$ each one located at a site of $\mathbb{Z}^d$.
The two error terms E_1 and E_2 can be described in the following way:

- the term E_1 comes from the fact that we neglected the possibility that the spectrum above energy λ can be created by many sites at the same time. That is from the fact that we neglected the possibility that more than a single random variable takes a value larger than λ.
- the second term E_2 comes from the fact that we neglected the tunneling between two sites k and k' at which the random variables take values close to λ.

2.1.1. *Asymptotic expansions in the classical regime.* Let us now assume that H is of finite range i.e. that $\hat{H}$ is a trigonometric polynomial. In this case, under more restrictive assumptions on H and F, we are able to get an asymptotic expansion of N. Therefore we need an assumption on H to control the tunneling. We won't describe it here and just refer to [4]. This assumption is automatically satisfied in dimension1 or if H is the discrete Laplacian.
To get an asymptotic expansion for N, we also need a better knowledge of $F(\lambda)$, so we assume

- all the moments of the i.i.d random variables $(\omega_k)_{k\in\mathbb{Z}^d}$ are finite (i.e. $\forall n \in \mathbb{N}$, $\mathbb{E}(|\omega_0|^n) < +\infty$).
- g admits a twice differentiable asymptotic expansion near $+\infty$: for some $\alpha > 0$ and $g_0^0 > 0$,

$$g(\lambda) \underset{\lambda\to+\infty}{\sim} \sum_{k\geq 0} g_k^0 \lambda^{\alpha(1-k)} + \ln\lambda \sum_{k\geq 0} g_k^1 \lambda^{-k}. \tag{7}$$

Then we have the

Theorem 2.3. *For H_ω and N defined as above, one has*

- *if $\alpha \leq 3$ then, one has*

$$\begin{aligned}\ln N(\lambda) \underset{\lambda\to+\infty}{\sim} & -g_0^0\lambda^\alpha + g_0^0\alpha h_0 \lambda^{\alpha-1} + g_0^0\alpha\left(\sum_{k\neq 0}|h_k|^2 - \frac{\alpha-1}{2}h_0^2\right)\lambda^{\alpha-2} + \\ & + n_3 - g_0^1\ln\lambda - g_1^0 + \sum_{\substack{i,j,m\geq 0\\ i+j+m\geq 1}} n_{i,j,m}\lambda^{-i-\alpha j}\left(\frac{\ln\lambda}{\lambda}\right)^m\end{aligned} \tag{8}$$

- *if $\alpha > 3$ then, one has*

$$\begin{aligned}\ln N(\lambda) \underset{\lambda\to+\infty}{\sim} & \sum_{\substack{j,l\geq 0\\ 0\leq 2j\alpha+l(\alpha-1)\leq\alpha(\alpha-1)}} n_{l,j}\lambda^{\alpha-l-\frac{2j\alpha}{\alpha-1}} - g_0^1\ln\lambda - g_1^0 + \\ & + \sum_{\substack{i,j,l,m,p\geq 0\\ i+j+l+m+p\geq 1\\ \alpha(\alpha-1)<\alpha(\alpha-1)i+(\alpha-1)l+2j}} n_{i,j,l,m,p}\lambda^{\alpha(1-i)-l-\frac{2j}{\alpha-1}}\left(\frac{\ln\lambda}{\lambda^{\tilde\alpha}}\right)^{m+p\alpha}\end{aligned} \tag{9}$$

  where
  - $\tilde\alpha = \frac{2\alpha}{\alpha-1}\left(\frac{\alpha-1}{2} - \left[\frac{\alpha-1}{2}\right]\right)$ *if* $\alpha \notin 2\mathbb{N}+1$, *and* $\tilde\alpha = \frac{2\alpha}{\alpha-1}$ *if* $\alpha \in 2\mathbb{N}+1$.
  - $n_{0,0} = -g_0^0$, $n_{1,0} = g_0^0\alpha h_0$, $n_{2,0} = g_0^0\alpha\sum_{k\neq 0}|h_k|^2 - g_0^0\frac{\alpha(\alpha-1)}{2}h_0^2$.
  - $n_{0,j} = n_{1,j} = 0$ *for any* j, $n_{2,1} = g_0^0(\alpha-1)\sum_{k\neq 0}|h_k|^{2\frac{\alpha}{\alpha-1}}$.

Remark 2.1. Theorem 2.3 shows that in Theorem 2.2, $\delta(\lambda)$ can not be taken in general of size $O(1/\lambda)$.
In the case when $F(t) = e^{-t^\alpha}$, the first terms of the asymptotics given in Theorem 2.3 were announced in [8].

Let us now comment on the results of Theorem 2.3. We can compare the different asymptotic expansions one gets when α is increasing. One sees that, with α increasing, new terms appear in the asymptotic expansion. These new terms carry the interaction (i.e. the tunneling) between the different sites in the lattice. The different terms of the principal part of the expansion may be described in the following way:

- the terms in $\lambda^{\alpha-j}$ $(j \in \mathbb{N})$ come essentially from the interaction between a site k and itself. It is essentially the asymptotic of the probability distribution of the highest eigenvalue of the operator $H + \omega_0\Pi_0$.

- the first new term, the term of order $\lambda^{\alpha-2-\frac{2}{\alpha-1}}$, comes from the larger probability of tunneling between one site and its neighbors when the random variables located at these sites both take large values. The other terms in $\lambda^{\alpha-2-\frac{2j}{\alpha-1}}$ come from tunneling between one site and its more remote neighbors. The index j is counting how far away from each other the sites are.

As $\alpha \to +\infty$, one notices that $\alpha - 2 - \frac{2}{\alpha-1} \sim \alpha - 2$. Hence the correction terms become more and more important. This underlines the already noticed fact that, as g'/g tends to 0 in a slower way, the possible tunneling between neighbors affects more and more the behavior of N. Hence, N behaves more and more in a quantum way.

To compare Theorem 2.3 to Theorem 2.2, we rewrite (9) in the same form as (6), if $\alpha > 2$, we get

$$\ln N(\lambda) = \ln F(\lambda + a_0 + a_1/\lambda + b_1\lambda^{-(\alpha+1)/(\alpha-1)} + o(\lambda^{-(\alpha+1)/(\alpha-1)})).$$

Comparing this with (6) and the analysis of (6) given after Theorem 2.2, we see that the principal correction to $I^{-1}(\lambda)$ is of order $\lambda^{-(\alpha+1)/(\alpha-1)}$. This order is increasing with α i.e. the decay of F.

To get a stronger quantum phenomenon, let us g grows faster than a polynomial at $+\infty$. To make the results simple, we assume that, for some $\alpha \in (0,1)$ and λ large enough, we have

$$g(\lambda) = g_0 e^{\lambda^\alpha}.$$

Then, we have the

Theorem 2.4. *For g as above, we have*

$$\ln N(\lambda) = \ln F(\lambda + h_0 + a\lambda^{\alpha-1} + o(\lambda^{\alpha-1})) \quad \textit{where} \quad a = \alpha g_0 \sum_{k\neq 0} |h_k|^2.$$

It is clear from Theorem 2.4 why the asymptotics given by Theorem 2.2 breaks down in the classical case when g'/g tends to 0 too slowly: the correction term we saw propagating upwards in the asymptotics in Theorem 2.3 has now overcome the correction computed in Theorem 2.2 i.e it is the error terms in this expansion that now become principal.

2.2. **The quantum regime.** We will say that we are in the quantum regime if

$$\frac{g'(\lambda)}{g(\lambda)} \underset{\lambda\to+\infty}{\to} +\infty. \tag{10}$$

It will be convenient to introduce $h = \ln g$. Then h is increasing and tends to $+\infty$ at $+\infty$. (10) becomes $h'(\lambda) \to +\infty$ as $\lambda \to +\infty$. To prove our result, we will need to assume that:

(1) $\hat{H}$ has a single maximum and this maximum is non-degenerate.
(2) for λ large enough, h' is increasing, differentiable and

$$-\left(\frac{1}{h'}\right)'(\lambda) = \frac{h''(\lambda)}{(h'(\lambda))^2} = \underset{\lambda\to+\infty}{\to} 0.$$

Assumption 1 is clearly fulfilled if $\hat{H}$ is the discrete Laplacian. As in [3], we could have relaxed the assumption on $\hat{H}$ and have assumed that it reaches its maxima at isolated points.
Assumption (2) just means that h' does not behave too wildly near $+\infty$.

Theorem 2.5. *In the quantum regime, under the above assumptions on $\hat{H}$, we have, when $\lambda \to +\infty$,*

$$\ln|\ln N(\lambda)| = \ln|\ln F(\lambda - \hat{H}_+)| + \frac{d}{2}\ln\left(\frac{F'(\lambda - \hat{H}_+)}{F(\lambda - \hat{H}_+)\ln F(\lambda - \hat{H}_+)}\right)(1 + o(1)).$$

The first correction to F is the shift of the energy λ by $-\hat{H}_+$. Notice that, in the classical regime, there was also a shift in energy but only by an amount $-\hat{H}_0$. The new shift increases the value of N as $-\hat{H}_+ < -\hat{H}_0$.

The second correction is due to the tunneling between many sites where the random variables take a value larger than $\lambda - \hat{H}_+$. This effect is of purely quantum nature: it is the same effect as the one discovered by I. Lifshitz at the edges of the spectrum when the support of the random variables $(\omega_k)_{k\in\mathbb{Z}^d}$ is compact (see [5], [6], [7]).

The coefficient $d/2$ appearing above is nothing but the exponent giving the decay of the density of states of H at the upper edge of its spectrum. In case we replace $\hat{H}$ by some analytic function, say $\hat{H}_0$, that has a degenerate critical point at its maximum, we expect the coefficient $d/2$ to be replaced by the exponent giving the decay of the density of states of H_0 at upper edge of its spectrum. This was proved in some simple cases for Lifshitz tails ([3]).

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Some variants of stochastic homogenization and their relation to random lattices

Claude Le Bris

The presentation is based on a series of joint works [1, 2, 3, 4] with Xavier Blanc (University Paris 6) and Pierre-Louis Lions (Collège de France and University Paris-Dauphine).

We study homogenization for scalar elliptic equations in divergence form with random coefficients:

$$-\operatorname{div}\left[A_\varepsilon\left(x,\omega\right)\nabla u(x,\omega)\right]=f.$$

In this context, our purpose is two-fold.

Our first purpose is to slightly extend the usual ergodic stationary setting, considering specific cases of random coefficients $A_\varepsilon\left(x,\omega\right)$, mainly of the form $A_\varepsilon\left(x,\omega\right)=A\left(\frac{x}{\varepsilon},\omega\right)$, not covered by the existing theories. These coefficients are typically obtained using random deformations of periodic coefficients. A prototypical case of such coefficients reads $A\left(\frac{x}{\varepsilon},\omega\right)=A_{per}\left(\Phi^{-1}\left(\frac{x}{\varepsilon},\omega\right)\right)$, where A_{per} is $\mathbb{Z}^d$-periodic, and Φ is almost surely a diffeomorphism. Its gradient $\nabla\Phi$ is assumed stationary in the sense

$$\forall k\in\mathbb{Z}^d,\quad \nabla\Phi(x+k,\omega)=\nabla\Phi(x,\tau_k\omega)\text{ almost everywhere in }x,\text{ almost surely,}$$

for a certain ergodic group action τ. The above setting has been introduced in [2]. Several variants are possible. They all allow for *explicit* homogenization results. That is, we are able to prove homogenization holds and identify the homogenized limit, using correctors problems, which are shown to be well-posed.

Our second purpose is to clarify the relation between the above questions of homogenization theory and our long term endeavour to define the energy of an infinite set of point particles in interaction, as exposed in [1, 3]. The problem under consideration can be phrased as follows: If we are given an infinite set of points x_i, say interacting with the two-body potential $W(x_i-x_j)$, it is an easy exercise to define the notion of *energy per particle* of this assembly of particles when the x_i are periodically arranged. On the other hand, when the position of the particles are more general, defining the energy per particle is a challenging question. In [1, 3], we addressed that latter question, respectively for some "general" deterministic sets of points, and for sets of random points. The point was to determine the appropriate geometric properties that allow for defining the energy. It turns out the properties we exhibited for that purpose have their counterpart in homogenization theory. More mathematically, the positions x_i may be used to define, using a construction introduced in [1], an appropriate algebra of functions, namely the smallest algebra, closed for some uniform norm on $\mathbb{R}^d$ (say L^∞), containing functions of the form

$$a(x)=\sum_{i_1\in\mathbb{N}}\sum_{i_2\in\mathbb{N}}\cdots\sum_{i_n\in\mathbb{N}}\varphi(x-x_{i_1},x-x_{i_2},\ldots,x-x_{i_n}).$$

Taking the entries A_{ij} of the matrix A in this algebra, one may then ask the question of elliptic homogenization within this algebra. Using this construction, we establish a correspondence between the homogenization problem and the, apparently distant, problem of definition of energies for sets of point particles.

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Stability and instability of Matter

Jan Philip Solovej

This talk was a review on the subject of the thermodynamics of charged quantum systems highlighting some of the main results from the past 40 years of research in this area. A more detailed written account can be found in the review [19] (see also the reviews [7, 9, 8]).

The main topics reviewed were stability of matter and existence of the thermodynamic limit for fermionic systems and instability for bosonic systems.

The existence of the thermodynamic limit states that the energy per volume has a limit as the volume tends to infinity. The relevans of this notion goes back to Onsager [17] and Fisher and Ruelle [6]. That existence of the thermodynamic limit holds for charged quantum gases consisting of fermionic particles were proved by Lieb and Lebowitz [10].

An important input is stability of matter stating that the energy per particle is bounded uniformly in the particle number. This was proved in the seminal work by Dyson and Lenard [3]. In [15] Lieb and Thirring gave a new proof of stability of matter relying on an inequality for the kinetic energy of fermions, known today as the Lieb-Thirring inequality.

These results were for non-relativistic particles with electro static interactions.

Stability of matter can be generalized in several ways. Relativistic effects can be included [16]. The particles may have classical electromagnetic interactions [4, 12] and one may consider relativistic effects together with classical electromagnetic interactions [13].

Finally, different attempts have been made at quantizing the electromagnetic field. In [5] non-relativistic particles interacting with a quantized field are considered and in [11] relativistic dynamics of the particles is included.

As the last point in the review it was discussed what happens if the particles are not fermionic. Dyson proved in [2] that a charged Bose gas is thermodynamically

unstable. He proved that the energy in the limit as the particle number goes to infinity behaves at least like the particle number to the power 7/5. Dyson, indeed, conjectured the exact asymptotic behavior. Conlon Lieb and Yau [1] proved that the power 7/5 was exact. Dyson's conjecture was eventually proved in [14, 18].

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Discrete dynamic models for phase transitions

Johannes Zimmer
(joint work with Hartmut Schwetlick)

The problem under consideration is easy to formulate. Consider a one-dimensional chain of atoms $\{q_j\}_{j\in\mathcal{Z}}$ on a torus ($\mathcal{Z} := \mathbb{Z}/L\mathbb{Z}$ with $L \in \mathbb{N}$) or on the real line ($\mathcal{Z} := \mathbb{Z}$). For each atom, the deformation is given by $u_k \colon \mathbb{R} \to \mathbb{R}$. The equations of motion are governed by Newton's law, which, in suitable units, reads

$$\ddot{u}_k(t) = V'(u_{k+1}(t) - u_k(t)) - V'(u_k(t) - u_{k-1}(t)) \tag{1}$$

for every $k \in \mathcal{Z}$ (on the torus, indices are counted modulo L). This is a spatially discretized, one-dimensional version of the well-studied equations of motions of an elastic material

$$u_{tt}(x) = \mathrm{Div}(\sigma(Du(x))). \tag{2}$$

Discretized equations as (1) are intrinsically interesting, as they correspond to forward-backward equations. This become apparent in the travelling wave formulation

$$u_j(t) = u(j - ct) \text{ for } j \in \mathcal{Z}, \tag{3}$$

since then Equation (1) transforms into

$$c^2\ddot{u}(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)). \tag{4}$$

This is the Euler-Lagrange function for the action functional

$$\phi(u) := \int_{\mathbb{R}} \left[\tfrac{1}{2}c^2\dot{u}(t)^2 - V(u(t+1) - u(t))\right] \mathrm{d}t.$$

Many problems, such models of crystal lattices, photonic structures, and Josephson junctions, can be described by lattice differential equations, of which (4) is one instance. There are a number of mathematical problems associated with lattice differential equations in general. A number of interesting papers [1, 2, 3] give a good insight into this field.

Such spatially discrete models are of interest in mathematical material science. In that context, an additional challenge can occur, which is at the centre of the present investigation. Namely, to describe phase transitions in solids ("martensitic" phase transformations), the interaction potential V is assumed to be *non-convex*. For the naïve continuum limit (2) of Equation (1), this corresponds to an ill-posed elliptic-hyperbolic problem. The travelling wave ansatz (3) singles out solutions and allows us to gain insight into the motion of a phase boundary. The existence of travelling waves will have implications for the prediction of a *kinetic relation*, which relate the velocity of a phase boundary to a configurational force.

Here, the existence of travelling waves is analysed rigorously for a special case, namely nearest-neighbour interaction with a piecewise quadratic energy,

$$V(\epsilon) = \frac{1}{2}\min\{(\epsilon+1)^2, (\epsilon-1)^2\} \tag{5}$$

The aim is to investigate the existence of solutions to (4) with V given by (5). It is shown that on a torus of length L, the existence of solutions with the strain distribution

$$\epsilon > 0 \text{ on } (0, \tfrac{L}{2}) \text{ and } \epsilon < 0 \text{ on } (\tfrac{L}{2}, L) \tag{6}$$

depends on the wave speed c: for some velocities c, a solution exists, while for other velocities nonexistence of a solution with strain distribution (6) can be proved.

For the real line ($\mathcal{Z} := \mathbb{Z}$), the existence of heteroclinic waves with the strain distribution

$$\epsilon > 0 \text{ for } x > 0 \text{ and } \epsilon < 0 \text{ for } x < 0$$

can be proved rigorously for sufficiently large velocities below the wave speed 1. Previous results [4, 6] were formal in the sense that they relied on physical considerations, namely the so-called *causality principle for a steady-state solution* [5]. This approach addresses the issue of the non-integrability of the Fourier transform of potential solutions (with singularities stemming from zeros of the dispersion relation). It seems natural to request a rigorous mathematical framework for problems of this kind, and a sketch of how to address this issue was contributed for the particular problem under consideration.

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Probabilistic approaches to large systems of Bosons

Stefan Adams

We study the large-N behaviour of a system of N Brownian motions $B^{(1)}, \dots, B^{(N)}$, with time horizon $[0, \beta]$ in $\mathbb{R}^d$ confined in subsets $\Lambda_N \subset \mathbb{R}^d$, under the symmetrised measure

$$\mathbb{P}_N^{(\mathrm{sym})} = Z_N^{(\mathrm{sym})}(\beta)^{-1} \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda_N} \mathrm{d}x_1 \cdots \int_{\Lambda_N} \mathrm{d}x_N \bigotimes_{i=1}^{N} \mu_{x_i, x_{\sigma(i)}}^{\beta, N}. \tag{1}$$

Here $\mathfrak{S}_N$ is the set of permutations of $1, \dots, N$, $\mu_{x,y}^{\beta,N}$ is the Brownian bridge measure on the time interval $[0, \beta]$ with initial point $x \in \Lambda_N$ and terminal point $y \in \Lambda_N$ and confinement to stay in Λ_N, and $Z_N^{(\mathrm{sym})}(\beta)$ is the normalisation

$$Z_N^{(\mathrm{sym})}(\beta) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda_N} \mathrm{d}x_1 \cdots \int_{\Lambda_N} \mathrm{d}x_N \bigotimes_{i=1}^{N} \mu_{x_i, x_{\sigma(i)}}^{\beta, N}(\Omega_\beta^N),$$

where Ω_β is the set of continuous functions $[0, \beta] \to \mathbb{R}^d$. Hence, the terminal location of the i-th motion is affixed to the initial location of the $\sigma(i)$-th motion, where σ is a uniformly distributed random permutation. That is, in (1) we have two random mechanisms. First we pick uniformly a permutation and after that we pick N initial points in Λ_N which are permuted according to the chosen permutation to obtain N terminal points. Then these N initial and terminal points determine the N random processes. Finally we average over all permutations and integrate over all initial points in the set Λ_N. Beside the fact that the symmetrised measure $\mathbb{P}_N^{(\mathrm{sym})}$ is itself of interest, there are two main motivations in studying the symmetrised measure.

The main motivation for studying the symmetrised measure $\mathbb{P}_N^{(\mathrm{sym})}$ stems from the applications of Feynman-Kac formulae to express thermodynamic functions in quantum statistical mechanics.

Let $\Lambda_N \subset \mathbb{R}^d$ a sequence of subsets with $N/|\Lambda_N| \to \rho \in (0, \infty)$ as $N \to \infty$. We are going to study large deviations for the empirical path measure

$$L_N = \frac{1}{N} \sum_{i=1}^{N} \delta_{B^{(i)}},$$

which we conceive as a Ω_β^N-measurable random probability measure in $\mathcal{M}_1(\Omega)$, where Ω is the set of all continuous paths $[0, \infty) \to \mathbb{R}^d$, under the symmetrised measure $\mathbb{P}_N^{(\mathrm{sym})}$. To prove large deviations principles under the symmetrised measure (1) one cannot proceed as in the Gärtner-Ellis-Theorem. A first approach is [6] and [7] for a different symmetrised measure. However, to see the peculiar correlations due to the symmetrisation one has to study the cycle structure for any permutation. The cycle structure allows to concatenate different Brownian motions to Brownian bridges with larger time horizon.

The cycle structure allows to replace the sum over permutations by a sum of integer partitions. For any integer N, a partition λ of N is the collection of integers

$n_1 \geq n_2 \geq \cdots \geq n_k \geq 1, k \in \{1, \ldots, N\}$, such that $\sum_{i=1}^{k} n_i = N$. We denote the set of all partitions of N by $\mathcal{P}_N$. Any partition $\lambda \in \mathcal{P}_N$ is determined by the sequence $\{r_k\}_{k=1}^{N}$ of positive integers r_k such that $\sum_{k=1}^{N} k r_k = N$, where we write $r_k(\lambda) = r_k$. We call the number r_k an *occupation number* of the partition. A cycle of length k is a chain of permutations, such as 1 goes to 2, 2 goes to 3, 3 goes to 4, etc. until $k-1$ goes to k and finally k goes to 1. A permutation with exactly r_k cycles of length k is said to be of type $\{r_k\}_{k=1}^{N}$. Hence, each partition $\lambda \in \mathcal{P}_N$ corresponds to a conjugacy class of permutations, i.e., those of the same type, with $N!/(\prod_{k=1}^{N} r_k! k^{r_k})$ elements.

The rate function of the large deviations principle is given as a variational formula involving an entropy functional and a Fenchel-Legendre transform. The entropy term

$$\mathcal{S}(Q) = \sum_{k=1}^{\infty} \widehat{Q}(k) \Big(\log \frac{\widehat{Q}(k)}{\widehat{Q}^*(k)} - 1 \Big)$$

for $Q \in \mathcal{M} = \{Q \in [0,1]^{\mathbb{N}} \colon \sum_{l \in \mathbb{N}} Q(l) = 1, Q(l) \geq Q(l+1) \, \forall l \in \mathbb{N}\}$, governs the large-$N$ behaviour of discrete shape measures of integer partitions. The rate functions is

$$I^{(\mathrm{sym})}(\mu) = \inf_{Q \in \mathcal{M}} \Big\{ \mathcal{S}(Q) + I^{(Q)}(\mu) \Big\} - \chi(\beta, \rho), \quad \mu \in \mathcal{M}_1(\Omega),$$

where

$$I^{(Q)}(\mu) = \sup_{F \in \mathcal{C}_{\mathrm{b}}(\Omega)} \Big\{ \langle F, \mu \rangle - \sum_{k \in \mathbb{N}} \widehat{Q}(k) \log \mathbb{E}_{0,0}^{k\beta} \Big(\mathrm{e}^{F(B)} \Big) \Big\}.$$

We provide a variational formula for the thermodynamic limit of the normalisation $Z_N^{(\mathrm{sym})}(\beta)$, which gives a variational expression for the specific free energy. A phase transition, i.e., a singularity of the free energy, exists for dimensions $d \geq 3$ depending on the density ρ and β. For high density, respectively for long time horizons $[0, \beta]$, the specific free energy is independent of the density.

Our main results give a phase transition for the empirical path measure. Let the set

$$A_k = \{\omega \otimes_{k\beta} \xi \colon \omega \in \Omega_k, \omega(0) = \omega(k\beta), \xi \in \Omega\},$$

where Ω_k is the set of paths $[0, k\beta] \to \mathbb{R}^d$, be given. The empirical path measure for dimensions $d = 1, 2$, and $\rho < \infty$, or $\rho < \rho_c$ for $d \geq 3$ has support on paths in any A_k, where one can insert any finite number of Brownian motions with time horizon $[0, \beta]$, i.e., for any $k \in \mathbb{N}$ one can concatenate exactly k Brownian motions to paths $\omega \in A_k$. This is due to the cycle structure of the permutations and the Lebesgue integration over all initial points in the definition of the symmetrised measure $\mathbb{P}_N^{(\mathrm{sym})}$. If the density ρ is high enough for $d \geq 3$, i.e., $\rho > \rho_c$ (or equivalently, if the inverse temperature is sufficiently large for given density, i.e., $\beta > \beta_c$, for $d \geq 3$), the mean path measure has positive weight on paths with an infinite time horizon, that is, concatenation of any finite number of Brownian motions with time horizon $[0, \beta]$ to obtain paths in the A_k's, is not sufficient. The excess density $(\rho - \rho_c)$ of Brownian motions with time horizon $[0, \beta]$ concatenate to infinite long cycles.

Hence, we have an empirical path measure interpretation of Bose-Einstein condensation. This novel interpretation adds to the existing notions of Bose-Einstein condensation ([8]), and allows to study systems of interacting Brownian motions. Future work will be devoted to this case [2]. Interacting Brownian motions in trap potentials have been so far analysed without symmetrisation, in particular, finite systems for vanishing temperature in [4] and large systems of interacting motions for fixed positive temperature in [5].

Scaling limits for shape measures of integer partitions in $\mathcal{P}_N$ under uniform distribution are obtained in [9].

Finally we review briefly the result in [5], where in collaboration with Bru and König we study a model of N mutually repellent Brownian motions under confinement to stay in some bounded region of space. Our model is defined in terms of a transformed path measure under a trap Hamiltonian, which prevents the motions from escaping to infinity, and a pair-interaction Hamiltonian, which imposes a repellency of the N paths. In fact, this interaction is an N-dependent regularisation of the Brownian intersection local times, an object which is of interest in the theory of stochastic processes.

The time horizon is kept fixed. We analyse the model for diverging number of Brownian motions in terms of a large deviations principle. The resulting variational formula is the positive-temperature analogue of the well-known Gross-Pitaevskii formula, which approximates the ground state of a certain dilute large quantum system; the kinetic energy term of that formula is replaced by a probabilistic energy functional.

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Interaction of singular limits and heterogeneities

Nicolas Dirr

1. Introduction

The derivation of effective models on "coarser" scales from models on a "finer" scale leads mathematically to the problem of finding a limit of a family of problems as the parameter ϵ, the ratio between the length-scales, tends to zero. This is often a *singular limits,* i.e. a situation where the limit of solutions to a family of problems solves a problem of a different type. One well-known example is the fact that solutions to the Allen-Cahn equation, a semi-linear evolution equation, converge under diffusive rescaling in a suitable sense to something which can be described by an interface moving by motion by mean curvature. Hence the type changes from a semi-linear PDE to a geometric evolution equation.

The Allen-Cahn equation is a gradient flow of a free-energy functional. The behaviour of this functional under a spatial rescaling has been studied by L. Modica and S. Mortola, [7], [6]. Again, the type of the functional changes: The approximating functionals F_ϵ are finite on any H^1-function, while the limit -in the sense of Γ-convergence in L^1- is finite only on those BV-functions which take values in the set $\{-1, 1\}$.

By taking into account *heterogeneities* on the small scale, one is lead to consider the interaction of a singular limit with the homogenisation of these heterogeneities. Unlike in "standard" homogenisation problems, there is no uniform ellipticity of the family of ϵ-problems.

2. Effective interfacial energy for a mesoscopic functional with periodic perturbation (Joint work Matteo Novaga, Pisa, and Marcello Lucia, Köln.)

Consider the free energy

$$G_\epsilon(u) := \int_\Omega \left[\epsilon |\nabla u|^2 + \frac{W(u)}{\epsilon} + \frac{1}{\epsilon^\alpha} f\left(\frac{x}{\epsilon^\alpha}\right) u \right] dx,$$

f periodic and mean zero and $1 \geq \alpha > 0$. W is a double-well potential with minima ± 1. Note that minimisers are not spatially constant, hence the minimal energy is negative and may, as $\epsilon \to 0$, diverge to $-\infty$, so we consider

$$F_\epsilon(u) = G_\epsilon(u) - \left(\inf_{H^1(\Omega)} G_\epsilon(\cdot) \right) \tag{1}$$

If f is symmetric under reflections across the coordinate axis and sufficiently small, then the limit yields an anisotropic surface energy. The effective surface tension can be obtained by solving a sequence of minimum problems over larger and larger cubes. In the case $0 < \alpha < 1$ these minimum problems are equivalent to homogenising an area functional with periodic perturbations, i.e. a separation between the singular limit and the homogenisation problem is possible.

Related problems have been studied by N. Ansini, A. Braides, V. Chiadò-Piat and C. Zeppieri, [1], [2].

3. Sharp-interface limit of a mesoscopic free energy with a random external field (Joint work with Enza Orlandi, Roma III)

Consider the functional

$$G_\epsilon(u) := \int_\Omega \left[\epsilon |\nabla u|^2 + \frac{W(u)}{\epsilon} + \frac{\theta(\epsilon)}{\epsilon} g_\epsilon(x,\omega)\, u \right] dx,$$

g_ϵ is a random field bounded in L^∞ with correlation length ϵ and mean zero, and W is a double-well potential with minima ± 1. Note that again minimisers are not spatially constant, so we have to subtract the minimal energy. In the random case small fluctuations can add up over large regions, so it is not trivial to show that there are essentially two minimisers, close to $+1$ and -1 respectively

We show for θ nonnegative and sufficiently small, but not necessarily vanishing as $\epsilon \to 0$, that the energy is bounded from below by a suitably coarse-grained energy that depends only on the averages of u in cubes of side-length ϵ. (Contour reduction)

In the special case $\theta(\epsilon) \sim [\log(1/\epsilon)]^{-1}$ we can use well-known techniques developed for the random field Ising model in order to show that there are two minimisers and to derive some of their properties. Moreover we show the Γ-convergence of F_ϵ (see (1)) to the area functional with a constant surface tension.

Thus at the highest order the randomness in the original model does not seem to play a role. But we present a formal argument stating that the interface undergoes oscillations that are smaller than the macroscopic scale, but are much larger than the correlation length ϵ. This feature is not present in the periodic or unperturbed case.

4. Dynamics: Interfaces in a heterogeneous medium

We consider an interface in a periodic environment, evolving by forced mean curvature flow. The forcing consists of a *constant* driving force F and a *periodic* forcing as in the cases considered above.

If the interface is a *graph* of a function with small gradients, this evolution law is well approximated by a semi-linear evolution equation.

For this semi-linear evolution equation we have shown in a joint paper with N.K. Yip, [5], that there exists a critical forcing $F_* > 0$ such that for any $0 \le F \le F_*$ there exists a periodic stationary solution called *pinning state*, while for $F > F_*$, there exist *pulsating wave solutions*.

We mention some possible extensions to the case of *random* obstacles. (Work in progress with J. Coville and S. Luckhaus.)

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The Thermodynamic Limit of Quantum Coulomb Systems

Mathieu Lewin
(joint work with Christian Hainzl and Jan Philip Solovej)

Ordinary matter is composed of electrons (charge -1) and nuclei (charge $+1$) interacting via Coulomb forces. The potential between two such particles of charges z and z' located at x and x' in $\mathbb{R}^3$ is

$$\frac{zz'}{|x-x'|}.$$

There are two difficulties which occur when trying to describe physical systems composed of electrons and nuclei.

The first is the singularity of $1/|x|$ at 0. It is necessary to explain why a particle will not rush to a particle of the opposite charge. In non-relativistic quantum mechanics, this is solved by Kato's inequality $|x|^{-1} \leq \epsilon(-\Delta) + C/\epsilon$, $\forall \epsilon > 0$, which is a consequence of the critical Sobolev embedding $H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$. It allows to control the Coulomb potential by the kinetic energy, proving what is usually called *stability of the first kind* [9, 10].

The second issue concerns the slow decay of $1/|x|$ at infinity and this has to do with the macroscopic behavior of quantum Coulomb systems. It is indeed necessary to explain how a very large number of electrons and nuclei can stay bounded together to form macroscopic systems, although each particle interacts with a lot of other charged particles due to the long tail of the interaction potential. Denote by $E(N)$ the ground state energy of a system of N particles (or $E(\Omega)$ the ground state energy of a system living in the domain Ω). The goal of the presentation was to explain how one can prove for some quantum systems that

$$E(N) \sim CN \text{ as } N \to \infty, \quad \text{or similarly} \quad E(\Omega) \sim C|\Omega| \text{ as } |\Omega| \to \infty \tag{1}$$

(usually $|\Omega|$ is of the same order as N). This behavior as the number of particles grows is mandatory to explain why matter do not collapse or explode in the thermodynamic limit. The constant C is then interpreted as the energy per particle (or per unit volume). A similar behavior can be proved for other quantities like the free energy in the non-zero temperature case.

The first step is to prove the inequality $E(N) \geq CN$ or $E(\Omega) \geq C|\Omega|$ which is usually referred to as *stability of matter* (or of the second kind) [9, 10]. This was first proved for quantum Coulomb systems by Dyson and Lenard [3, 4]. Another proof was given by Lieb and Thirring based on a functional inequality [13]. A

review of the results and techniques to prove stability of matter was done in a talk by Jan Philip SOLOVEJ during the workshop.

The existence of the above behavior (1) as $N \to \infty$ was proved first for quantum Coulomb systems by Lieb and Lebowitz in [11] for a system containing electrons and nuclei both considered as quantum particles, hence invariant by rotation. Fefferman gave a different proof [5] for the case where the nuclei are classical particles placed on a lattice, a system which is not invariant by rotation.

In the talk, I presented a different method [8] which is sufficiently general to apply to the case treated by Lieb and Lebowitz, the crystal tackled by Fefferman, and other quantum Coulomb systems which were not studied before. Our method is based on an electrostatic inequality of Graf and Schenker [6] which itself was inspired by ideas of Conlon, Lieb and Yau [2]. It allows to estimate from below the total Coulomb energy of a system of charged particles in a domain by the sum of the Coulomb energies of the particles in smaller domains (simplices) which completely tile the bigger domain. This inequality allows to take into account the subtle screening effects which are present in ordinary matter and which are so difficult to quantize.

A much more difficult task is to prove the convergence of *states* in the thermodynamic limit. This was done for simpler models of Thomas-Fermi type [12] of Hartree-Fock type [1], in which the quantum state is described by a simpler object like the density or the density matrix. In [7], we could prove similar results for the Hartree-Fock approximation of QED. But this is still open for many-body systems.

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Definition of average energies for stochastic lattices

Xavier Blanc
(joint work with C. Le Bris & P.-L. Lions)

We consider the question of making a link between atomistic energies and (macroscopic) hyperelastic energies.

To fix the ideas, let us address this question in the most simple case, that is, the case of a two-body potential energy and periodic positions for the atoms. In this setting, a solid is defined by

(1) a reference *macroscopic* configuration $\mathcal{D}$ which is an open bounded subset of $\mathbb{R}^3$;
(2) a reference *microscopic* configuration which is a periodic lattice, say, $\mathbb{Z}^3$;
(3) a macroscopic deformation $u : \mathcal{D} \longrightarrow \mathbb{R}^3$ which is supposed to be a diffeomorphism.

In addition to the above hypotheses, we assume that the atomic positions in the deformed configuration are exactly $u(X_i)$, where the X_i are the reference positions. In other words, the deformation is *scale-independent*.

The energy is defined by a two-body potential W, which is assumed to be radially symmetric and decay fast at infinity. Then the microscopic energy per particle reads

$$\mathcal{E}_\varepsilon(u) = \frac{1}{2N} \sum_{i \neq j \in \mathbb{Z}^3 \cap \mathcal{D}} W\left(u(\varepsilon i) - u(\varepsilon j)\right),$$

where $N \approx \frac{|\mathcal{D}|}{\varepsilon^3}$ is the number of atoms. Assuming that the potential W reads $W(x) = W_0(\frac{x}{\varepsilon})$, which is a physically relevant hypothesis, we then have, using a simple computation,

$$\lim_{\varepsilon \to 0} \mathcal{E}_\varepsilon(u) = \frac{1}{2|\mathcal{D}|} \int_{\mathcal{D}} \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} W_0\left(\nabla u(x) k\right) dx, \tag{1}$$

which has the form of hyperelastic energies written in material science textbooks.

The talk is devoted to the study of extensions of the above simple computation:

(1) replace the periodicity assumption (2) above by the assumption that the atoms have stochastic stationary positions, and
(2) change the two-body energy for a Thomas-Fermi type model.

Constructing an adapted ergodic setting, we define accordingly the notion of stationarity. We then use it to carry out the macroscopic limit described above, both in the case of two-body energies and in the case of Thomas-Fermi energies.

In the course of the proof, the notion of thermodynamic limit naturally plays a central role. We therefore focus on this notion first, then on the problem of the corresponding macroscopic limit. To treat the case of Thomas-Fermi energies, we in particular need to prove uniqueness for systems of (stochastic) nonlinear elliptic partial differential equations.

Finally we mention some links between these problems and stochastic homogenization of linear second order elliptic equations. This work was published in [3].

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Localization and propagation in high contrast media via "non-classical" homogenization

Valery P. Smyshlyaev

(joint work with Ilia V. Kamotski)

One of physical motivations for the reported study is wave localization in photonic crystal fibers (PCF). Those are optical materials representing geometrically a periodic medium (whose physical properties vary across the fiber but not along it), with the defect being its "core", which is a propagating "channel" or a waveguide: electromagnetic waves of certain frequencies (the "band gap" frequencies) fail to propagate in the surrounding periodic medium and hence remain localized inside the PCF, which allows for them to propagate along the core for long distances with little loss. Mathematically, the problem reduces to an appropriate spectral problem at the cross-section of the PCF, cf. Figure 1. This is that of characterization of localized modes or eigenfunction (whenever such exist) in the band gaps in the Floquet-Bloch spectrum for the Maxwell's operator in the surrounding periodic medium with a fixed "propagation constant" (the wave vector along the fiber). Similar effects occur in elastic ("phononic") rather than optical (photonic) materials. The latter cross-sectional geometry is a periodic medium "perturbed" by a finite size heterogeneity (domain Ω_2 in Fig. 1). The problem is hence first in detecting the band gaps in the periodic medium without defects and then in finding, in the presence of a defect, the "extra point spectrum" in the gaps as well as the associated eigenfunctions, the localized states. In the present work we aim at detecting such localized modes in an asymptotically explicit way due to defects in high contrast periodic medium applying and appropriately developing further the tools of (high contrast) "non-classical" homogenization theory. In physical terms, we consider here a simplified model with scalar rather than Maxwell's or elasticity equations and with zero propagation constant, which captures the essence of the underlying effects:

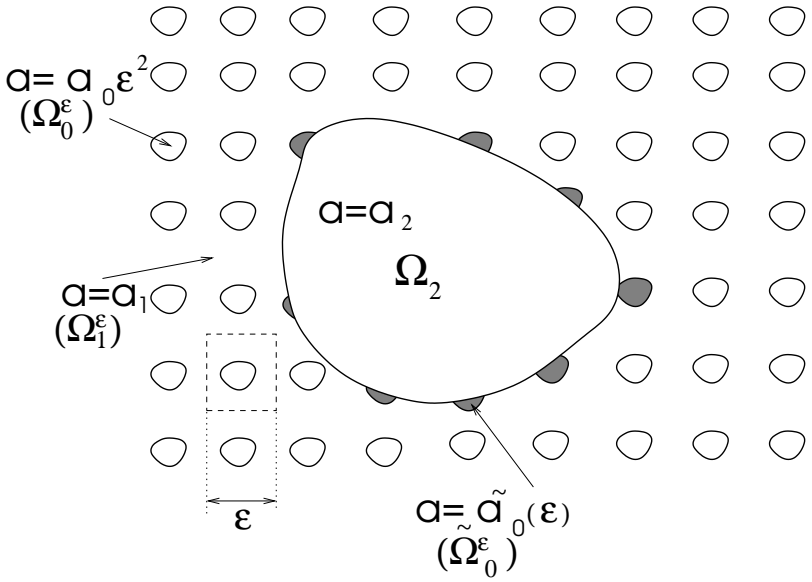

FIGURE 1. Geometric configuration: a defect in a rapidly oscillating high contrast medium

$$Au := -\nabla \cdot \Big((a(x) + b(x)) \nabla u \Big) = \lambda u,$$

which is a spectral problem for operator A, self-adjoint in $L^2(\mathbb{R}^n)$. Here $x \in \mathbb{R}^n$, $n \geq 2$, a and $a+b$ are strictly positive, a is n-periodic and b (related to the defect) is compactly supported.

Spectral theory ensures that the "unperturbed" operator ($b \equiv 0$) has a band structure, whose (essential) spectrum persists under the perturbation, so the only "extra" spectrum may be the point spectrum in the gaps, with corresponding eigenvalues exponentially decaying at infinity. If the size of the defect is much larger than that of the periodicity, one could hope to "homogenize" the periodicity when the underlying small parameter ε tends to zero. However, the "classical" homogenization is of no use in the present context since the homogenized operator (with constant coefficients) ceases having the band gap structure, effectively accounting only for the behaviour at the bottom of the spectrum of the original operator. We employ instead a *high contrast* ("non-classical") homogenization, introducing another small parameter of contrast δ. Such a situation is realized physically even for moderately contrast media when the propagation constant is close to a "critical" value. The limit behavior then depends on the relation between δ and ε, and one can see that there is only one "critical" scaling $\delta(\varepsilon) \sim \varepsilon^2$, the so-called "double-porosity" scaling, when the phenomena at the micro and macro scales are coupled in a non-trivial way, see [1] for precise details.

It then appears that the "limit" problem (in contrast to the classical homogenization) is "two-scale", and recently developed techniques of *two-scale convergence* appear an appropriate tool, see e.g. [2] for recent developments and further references therein. In particular, one can define a two-scale limit operator A_0, which is self-adjoint in a subspace of $L^2(\mathbb{R}^n \times Q)$ (Q in the periodicity cell in

the "fast" variable $y = x/\varepsilon$). The unperturbed part of the limit operator has an explicitly described band-gap structure, cf. [2]. In particular, the "macroscopic" part u_0 depends on the spectral parameter in a highly nonlinear way:

$$-\nabla \cdot \left(A^{hom} \nabla u_0 \right) = \beta(\lambda) u_0,$$

where A^{hom} is the standard "porous" homogenized matrix with void inclusions (i.e. infinite contrast), and $\beta(\lambda)$ is an explicit function introduced by Zhikov [2] whose values are negative in the gaps of the (defect free) limit operator and positive on its bands. We show that the perturbed limit operator may develop explicit extra point spectrum in the gaps [1]. We then prove [1, Thm 4.1] that, for small enough ε, near every eigenvalue λ_0 there exists an eigenvalue $\lambda(\varepsilon)$ of the original operator A_ε, with an error bound

$$|\lambda(\varepsilon) - \lambda_0| \leq C\, \varepsilon^{1/2}.$$

The proof employs a Rayleigh-type variational principle, with appropriately modified formal asymptotic approximations serving as test functions, and the above "ε-square-root" error bound is an effect of a boundary layer in the high-contrast homogenization, see [1] for the details.

Proof of the "converse" statement requires an additional analysis, advanced most recently by M. Cherdantsev [3]. This is based on establishing strong two-scale resolvent convergence of A_ε to A_0, supplemented further by certain (two-scale) compactness properties for the "pre-limit" operator A_ε. Namely, the normalized eigenfunctions u^ε of A_ε appear compact in the sense of strong two-scale convergence, and hence, up to a subsequence, strongly two-scale converge to a "non-trivial" element which may only be an eigenfunction of A_0. This implies that *all* the point spectrum converges to that of A_0 with appropriate multiplicities, etc. A central technical ingredient in achieving this is a results on a uniform exponential decay of u^ε, [3].

A very interesting related further issue is analysis of the asymptotic behavior of solutions in the "propagating" rather than "localizing" regimes, i.e. on the bands ($\beta(\lambda) > 0$) rather than in the gaps ($\beta(\lambda) < 0$) of the (defect free) limit operator. A formal calculation then shows that, sufficiently close to band ends, there is a high dispersion, with slow group velocity. This suggests the possibility of propagating in such (high contrast) media of wave packets with slow speed (cf. the so-called "slow light" effect). Microscopically, this may be related to the "coupled resonances" and "metastability" effects: the oscillations are restricted to the "soft" inclusions persisting there for a sufficiently large time but eventually passing over to the neighbouring oscillators, etc.

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Phase transitions in quantum spin systems

Marek Biskup

(joint work with Lincoln Chayes and Shannon Starr)

Recall that an SU(2) spin is a triplet of $2J+1$-dimensional self-adjoint matrices $\vec{S} = (S^1, S^2, S^2)$ that form an irreducible representation of the Lie algebra $\mathfrak{su}(2)$ on $\mathbb{C}^{2J+1}$ with commutation relations

$$[S^\alpha, S^\beta] = \mathrm{i}\epsilon^{\alpha\beta\gamma} S^\gamma,$$

where $\epsilon^{\alpha\beta\gamma}$ is the totally asymmetric tensor. The number J takes values in half integers, $J \in \{0, \frac{1}{2}, 1, \dots\}$. The representation is generally chosen so that S^3 is diagonal, $S^3 |M\rangle = M |M\rangle$, where $|M\rangle$, $M = -J, -J+1, \dots, J-1, J$, are basis vectors in $\mathbb{C}^{2J-1}$.

As usual, a collection of spins, indexed by the base set Λ, is described by product operators

$$\vec{S}_x = 1 \otimes \cdots \otimes 1 \otimes \vec{S} \otimes 1 \cdots \otimes 1$$

acting on the product Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda}(\mathbb{C}^{2J+1})$ in a natural way. Product and sums applied to these generate the algebra of observables.

Theoretical physicists generally believe that the quantum SU(2) spin systems with large largest weight J (the spin magnitude) behave essentially classically at positive temperatures. The most compelling mathematical evidence for this belief comes in the form of the Berezin-Lieb inequalities [5, 3]. These inequalities make ingenious use of coherent states which, for one spin, are vectors

$$|\Omega\rangle = \sum_{M=-J}^{J} \binom{2J}{J+M}^{1/2} [\cos(\theta/2)]^{J+M} [\sin(\theta/2)]^{J-M} \, \mathrm{e}^{\mathrm{i}(J-M)\phi} \, |M\rangle$$

indexed by points $\Omega = (\theta, \phi)$ on the unit sphere $\mathbb{S}_2$ in $\mathbb{R}^3$, to link the $J \to \infty$ limit of the free energy of the quantum model to the free energy of its the classical, $J = \infty$, counterpart. Explicitly, if A is a bounded operator on $\mathcal{H}_\Lambda$, we have

$$\int_{(\mathbb{S}_2)^{|\Lambda|}} \frac{\mathrm{d}\Omega}{(4\pi)^{|\Lambda|}} \, \mathrm{e}^{\langle A\rangle_\Omega} \le \frac{\mathrm{Tr}_{\mathcal{H}_\Lambda}(\mathrm{e}^A)}{(2J+1)^{|\Lambda|}} \le \int_{(\mathbb{S}_2)^{|\Lambda|}} \frac{\mathrm{d}\Omega}{(4\pi)^{|\Lambda|}} \, \mathrm{e}^{[A]_\Omega}, \tag{1}$$

where $\mathrm{d}\Omega = \prod_{x\in\Lambda} \mathrm{d}\Omega_x$ is the *a priori* measure on classical spin configurations, $\langle A\rangle_\Omega = \langle\Omega|A|\Omega\rangle$ is the lower symbol—relative to the product coherent state $|\Omega\rangle = \bigotimes_{x\in\Lambda} |\Omega_x\rangle$—while $[A]_\Omega$, the upper symbol, is a function $(\mathbb{S}_2)^{|\Lambda|} \to \mathbb{C}$ such that

$$A = \Bigl(\frac{2J+1}{4\pi}\Bigr)^{|\Lambda|} \int_{(\mathbb{S}_2)^{|\Lambda|}} \mathrm{d}\Omega \, [A]_\Omega \, |\Omega\rangle \, \langle\Omega|.$$

The natural choice for A is $A = -\beta H_\Lambda$ where H_Λ is the Hamiltonian in Λ; the bounds in Eq. (1) then show that the quantum free energy tends to that of (an appropriately extracted) classical systems in the limit $J \to \infty$.

While extremely illuminating, the control of the limiting free energy does not tell anything about the phase transitions in quantum system. This can be overcome by enhancing the Berezin-Lieb inequalities into *pointwise* bounds on the matrix elements of the Gibbs-Boltzmann weight $\mathrm{e}^{-\beta H}$ relative to coherent states.

Theorem 1. Suppose the Hamiltonian takes the form

$$H_\Lambda = \sum_{\Gamma\colon\, \Gamma\subset\Lambda} h_\Gamma$$

for some collection of self-adjoint operators h_Γ "depending" only on the spins in Γ subject to the following properties:

(1) (finite range) $\exists R > 0$ such that $h_\Gamma = 0$ if $|\Gamma| > R$.

(2) (bounded energy density)

$$c_1 := \sup_{x\in\Lambda} \sum_{\Gamma\colon\, \Gamma\ni x} \|h_\Gamma\| < \infty$$

(3) (Lipschitz continuity) Given the upper symbols $[h_\Gamma]_\Omega$, there exists $c_2 < \infty$ such that for all configurations $\Omega, \Omega' \in (\mathbb{S}_2)^\Lambda$,

$$\big|[h_\Gamma]_\Omega - [h_\Gamma]_{\Omega'}\big| \le c_2 \|\Omega - \Omega'\|_{L^2(\Lambda)}\, \|h_\Gamma\|.$$

Then there are constants $c, c' \in (0,\infty)$ depending only on c_1, c_2 and R such that if $\beta \le c'\sqrt{J}$ then for each $\Omega \in (\mathbb{S}_2)^\Lambda$,

$$\big(\mathrm{e}^{-\beta\langle H_\Lambda\rangle_\Omega} \le\big)\ \langle\Omega|\mathrm{e}^{-\beta H_\Lambda}|\Omega\rangle \le \mathrm{e}^{-\beta[H_\Lambda]_\Omega + c|\Lambda|\beta/\sqrt{J}} \tag{2}$$

The significance of Eq. (2) resides in the ensuing comparison of quantum and classical expectations: Given a classical event $\mathcal{A} \subset (\mathbb{S}_2)^\Lambda$, let

$$Q_\mathcal{A} = \Big(\frac{2J+1}{4\pi}\Big)^{|\Lambda|} \int_\mathcal{A} \mathrm{d}\Omega\ \ |\Omega\rangle\,\langle\Omega|$$

be a quantum analogue of the classical indicator $1_\mathcal{A}$. Let $\langle - \rangle_{\beta,\Lambda}$ be the usual quantum Gibbs-Boltzmann state,

$$\langle A\rangle_{\beta,\Lambda} = \frac{\mathrm{Tr}(A\mathrm{e}^{-\beta H_\Lambda})}{\mathrm{Tr}(\mathrm{e}^{-\beta H_\Lambda})},$$

and let $\mathbb{P}_{\beta,\Lambda}$ be the corresponding classical Gibbs (probability) measure at inverse temperature β defined using the Hamiltonian $[H_\Lambda]_\Omega$. If

$$\|[H_\Lambda] - \langle H_\Lambda\rangle\|_\infty \le \xi|\Lambda|$$

for some $\xi < \infty$, then Eq. (2) implies that for each $\mathcal{A} \subset (\mathbb{S}_2)^\Lambda$,

$$\big\langle Q_\mathcal{A}\big\rangle_{\beta,\Lambda} \le \mathrm{e}^{(\xi + 2c\beta/\sqrt{J})|\Lambda|}\mathbb{P}_{\beta,\Lambda}(\mathcal{A}). \tag{3}$$

For events $\mathcal{A}$ whose classical probability decays exponentially with $|\Lambda|$, this yields a non-trivial bound on the quantum expectation of $Q_\mathcal{A}$. Typically $\xi = O(1/J)$ so the error can be made as small as desired by taking J large.

Despite its rather crude nature, the inequality (3) is ideally suited for an application of chessboard estimates (cf Fröhlich and Lieb [4]). Indeed, the latter give a bound on the expectations of $Q_{\mathcal{A}}$ for $\mathcal{A}$ forcing a specific "bad" event $\mathcal{B}$ in m disjoint blocks—in a fixed partition of $\mathbb{Z}^d$—by the m-th power of partition-function per-block for the event that $\mathcal{B}$ occurs in *all* blocks. Since this involves large-deviation rate functions for events whose probabilities exponentially small in Λ, the prefactor $\mathrm{e}^{(\xi+2c\beta/\sqrt{J})|\Lambda|}$ in Eq. (3) provides only a finite multiplicative correction which is harmless provided the classical probability of $\mathcal{B}$ is small.

The meta-theorem that arises is that *the quantum spin system undergoes a similar phase transition as its classical counterpart, provided this transition occurs at inverse temperature β much smaller than a constant times $\sqrt{J}$.* This allows us to construct a proof of phase coexistence in a number of models—in particular, those with temperature-driven or order-by-disorder phase transitions—which have not been accessible via the exponential localization technique of Fröhlich and Lieb [4]. Details of the above theory, and the analysis of specific models, can be found in [2]; a recent review of chessboard estimates and their use is the subject of [1].

The bound in Theorem 1 is rather crude because it dominates everything by the worst-case possible overlap. One can speculate that a more-refined approach—involving, perhaps, a multiscale analysis—might offer a tool to avoid the use of reflection positivity (which is needed for chessboard estimates) from the analysis of the corresponding quantum system. This could help construct a proof of phase transitions in a number of quantum spin systems that have heretofore resisted rigorous methods; most notably, the quantum Heisenberg ferromagnet.

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Lieb-Robinson Bounds and Related Results

Robert Sims
(joint work with Bruno Nachtergaele, Yoshiko Ogata)

In 1972 Lieb and Robinson [7] proved a bound on the group velocity corresponding to certain quantum spin systems. These locality estimates apply to the dynamics generated by short range Hamiltonians and from them a variety of interesting consequences follow, see e.g. [2, 12]. In this short note, we will report on some recent advances concerning these results and discuss a few of their applications.

The Basic Set-Up:

The quantum spins systems we will be considering consist of a finite or infinite number of spins, labeled by $x \in V$. A finite dimensional Hilbert space $\mathcal{H}_x$ is assigned to each site $x \in V$. These may represent the spin of an electron, photon, or an atom. In other contexts, these states may represent the ground state and first exited state of an atom or a molecule. More abstractly, these systems may, for example, model a collection qubits, the basic units of quantum information theory and quantum computation.

If the set V is finite, the Hilbert space of states is given by $\mathcal{H}_V = \bigotimes_{x\in V} \mathcal{H}_x$. For each spin x, the observables are the complex $n_x \times n_x$ matrices, M_{n_x}, where $n_x = \dim(\mathcal{H}_x)$. In this context, the algebra of observables for the whole system is $\mathcal{A}_V = \bigotimes_{x\in V} M_{n_x}$.

The locality results we wish to describe pertain to observables with finite support. Here, the support of an observable is understood as follows. If $X \subset V$, we write $\mathcal{A}_X = \bigotimes_{x\in X} M_{n_x}$. By identifying $A \in \mathcal{A}_X$ with $A \otimes \mathbb{1} \in \mathcal{A}_V$, we have that $\mathcal{A}_X \subset \mathcal{A}_V$. Given $A \in \mathcal{A}_V$ for which $A = \tilde{A} \otimes \mathbb{1}$ with $\tilde{A} \in \mathcal{A}_X$ we say that the support of A is contained in X.

For infinite V, the algebra of observables is the completion of the algebra of local observables given by

$$\mathcal{A}_V = \bigcup_{X\subset V} \mathcal{A}_X$$

where the union is over all finite $X \subset V$.

Interactions and the Dynamics:

An interaction is a map Φ from the set of subsets of V to $\mathcal{A}_V$ with the property that $\Phi(X) \in \mathcal{A}_X$ and $\Phi(X) = \Phi(X)^*$ for all finite $X \subset V$. A quantum spin model is defined to be a family of Hamiltonians, parametrized by finite subsets $\Lambda \subset V$, given by

$$H_\Lambda^\Phi = \sum_{X\subset\Lambda} \Phi(X). \tag{1}$$

For notational convenience, we will often drop the dependence of H_Λ^Φ on Φ.

The dynamics, or time evolution, of a quantum spin model is the one-parameter group of automorphisms, $\{\tau_t\}_{t\in\mathbb{R}}$, defined by

$$\tau_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda}, \quad A \in \mathcal{A}_\Lambda, \tag{2}$$

which is always well defined for finite sets Λ. In the context of infinite systems, a boundedness condition on the interaction is required in order for the finite-volume dynamics to converge to a strongly continuous one-parameter group of automorphisms on $\mathcal{A}_V$.

To describe the interactions for which we can prove our locality results, we first put a condition on the set V; relevant only in the event that V is infinite. We assume that V is equipped with a metric d and that there exists a non-increasing function $F : [0, \infty) \to (0, \infty)$ for which:
i) F is uniformly integrable over V, i.e.,

$$\| F \| := \sup_{x \in V} \sum_{y \in V} F(d(x, y)) < \infty, \tag{3}$$

and

ii) F satisfies

$$C := \sup_{x,y \in V} \sum_{z \in V} \frac{F(d(x, z))\, F(d(z, y))}{F(d(x, y))} < \infty. \tag{4}$$

Given a set V equipped with a metric d, it is easy to see that if F satisfies i) and ii) above, then for any $a \geq 0$ the function

$$F_a(x) := e^{-ax} F(x), \tag{5}$$

also satisfies i) and ii) with $\|F_a\| \leq \|F\|$ and $C_a \leq C$.

To any set V for which there exists a function F satisfying i) and ii) above, we define the set $\mathcal{B}_a(V)$ to be those interactions Φ on V which satisfy

$$\|\Phi\|_a := \sup_{x,y \in V} \sum_{X \ni x,y} \frac{\|\Phi(X)\|}{F_a(d(x, y))} < \infty. \tag{6}$$

Lieb-Robinson Bounds and Some Comments:
In a recent series of works [3, 10, 4, 9], there have been some important improvements on the original Lieb-Robinson results, [7], see also [2, 12]. We will now state the version which appears in [9].

Theorem 1 (Lieb-Robinson Bound)**.** Let $a \geq 0$ and take $\Lambda \subset V$ a finite subset. Denote by τ_t^Λ the time evolution corresponding to a Hamiltonian

$$H_\Lambda = \sum_{X \subset \Lambda} \Phi(X) \tag{7}$$

defined in terms of an interaction $\Phi \in \mathcal{B}_a(V)$. There exists a function $g : \mathbb{R} \to [0, \infty)$ with the property that, given any pair of local observable $A \in \mathcal{A}_X$ and $B \in \mathcal{A}_Y$ with $X, Y \subset \Lambda$, one may estimate

$$\left\| [\tau_t^\Lambda(A), B] \right\| \leq \frac{2 \|A\| \, \|B\|}{C_a} g_a(t) \sum_{x \in X} \sum_{y \in Y} F_a(d(x, y)), \tag{8}$$

for any $t \in \mathbb{R}$. Here the function

$$g_a(t) = \begin{cases} \left(e^{2\,\|\Phi\|_a\, C_a\,|t|} - 1\right) & \text{if } d(X,Y) > 0, \\ e^{2\,\|\Phi\|_a\, C_a\,|t|} & \text{otherwise.} \end{cases} \tag{9}$$

A variety of comments are useful in interpreting this theorem. First, if $\Phi \in \mathcal{B}_a(V)$ for some $a > 0$, then the double sum appearing in (8) may be estimated trivially by

$$\sum_{x \in X} \sum_{y \in Y} F_a(d(x,y)) \leq \|F\| \, \min(|X|, |Y|)\, e^{-a d(X,Y)}. \tag{10}$$

Thus, we have that

$$\left\| [\tau_t^\Lambda(A), B] \right\| \leq \frac{2\,\|A\|\,\|B\|}{C_a} \, \|F\| \, \min(|X|, |Y|)\, e^{-a\left[d(X,Y) - \frac{2\|\Phi\|_a C_a}{a}|t|\right]}, \tag{11}$$

which corresponds to a velocity of propagation given by

$$V_\Phi := \inf_{a>0} \frac{2\|\Phi\|_a C_a}{a}. \tag{12}$$

Next, we observe that for fixed local observables A and B, the bounds above, (8) and (11), are independent of the volume $\Lambda \subset V$; given that Λ contains the supports of both A and B. Finally, we note that these bounds only require that one of the observables has finite support; in particular, if $|X| < \infty$ and $d(X,Y) > 0$, then the bounds are valid irrespective of the support of B.

Improvements and Applications:

The result stated in Theorem 1 above differs from that which may be found in [7] in three important ways. First, the new proof does not require the use of the Fourier transform and therefore extends to non-lattice (V, d). These results may be of interest then to those who wish to study quantum spin systems in the context of quasi-crystals. Next, our results allow for sufficiently fast polynomial decay instead of just finite-range or exponentially decaying interactions. Hence, we can prove the existence of thermodynamic quantities for a larger class of interactions than was previously known [9]. Lastly, the constants which appear in our bound do not depend on the dimensions of the underlying, single-site Hilbert spaces.

We will now end with a brief mention of two recent applications of Theorem 1. The first concerns gapped Hamiltonians. In the physics literature the term *massive ground state* typically implies two properties: the existence of a *spectral gap* above the ground state energy and the *exponential decay* of spatial correlations in the ground state. It has long been (correctly) believed that the first implies the second and often also (incorrectly) that the second implies the first, see [8] for a simple counter-example involving valence bond states. Exponential clustering, i.e., the fact that the existence of a spectral gap implies exponential decay of correlations in the ground state, has recently been proven using these locality bounds, see [10, 4].

Lastly, we discuss a multi-dimensional version of the Lieb-Schultz-Mattis (LSM) Theorem. Perhaps one of the most interesting theorems contained in the paper by Lieb, Schultz, and Mattis [6], concerns the the spin-1/2 anti-ferromagnetic chain.

The anti-ferromagnetic spin chain is a one-dimensional quantum spin system defined on the set of integers $\Lambda_L \subset [0, L]$ with $\mathcal{H}_x \cong \mathbb{C}^2$ for each $x \in \Lambda_L$. The Hamiltonian is given by

$$H_L = \sum_{x=1}^{L-1} \vec{S}_x \cdot \vec{S}_{x+1},$$

where $\vec{S}_x$ is the spin vector situated at site x whose components are simply the Pauli spin matrices. The LSM Theorem states that *if the ground state of H_L is unique, then the gap to the first exited state is bounded by C/L.* This result was later generalized to other one dimensional models by Affleck and Lieb in [1]. A result of Lieb and Mattis, [5], shows that for the particular model H_L with L even, the assumption (hence Theorem) is true.

Based on the ideas presented by Hastings in [3], we were recently able to provide a rigorous proof, see [11], of an analogue of the LSM Theorem for spin-1/2 anti-ferromagnetic models in arbitrary dimensions. Both the new Lieb-Robinson bounds and the exponential clustering theorem, discussed above, play a crucial role in estimating the energy of the variational state and proving its orthogonality to the ground state.

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Evolution of martensitic phase boundaries in heterogeneous media

Patrick W. Dondl

The motivation for this problem lies in the question of whether, and how, hysteresis can arise from a linear microscopic kinetic relation through the effect of defects such as precipitates in the medium. Hysteresis in the physical problems considered stems from a stick-slip behavior of phase boundaries with respect to an applied force; this behavior is therefore often assumed in macroscopic models. The goal of my research is to show how it arises through homogenization from the interplay of a linear microscopic evolution law with the heterogeneities that are always present in a physical material.

For the basic model we consider an elastic solid occupying a domain Ω with a bulk energy of the form

$$\mathcal{F}_{\text{elastic}} = \int_\Omega W(\nabla u, x), \tag{1}$$

where $u\colon \Omega \to \mathbb{R}^n$ is the displacement of the body. The domain is split into a subdomain E and its complement, separated by a phase boundary Γ—this represents the two phases the material can be in. There may also be inclusions $A = \bigcup_i A_i$ present in Ω. The elastic energy density $W(\nabla u, x)$ depends explicitly on the position x: its minimum, the transformation strain, is constant on the domains occupied by each phase or the inclusions and jumps across their respective boundaries. A surface energy of the form

$$\mathcal{F}_{\text{surface}} = c \int_\Omega |\nabla \chi_E| \tag{2}$$

penalizing the length of the phase boundary can also be added.

Assuming smoothness of the involved quantities, one can calculate the rate of change of the energy in the system, depending on the normal velocity v_n of the phase boundary, to be

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{F}_{\text{elastic}} + \mathcal{F}_{\text{surface}}\right) = -\int_\Gamma f\ v_n, \tag{3}$$

where f is the thermodynamic driving force. The goal is to analyze the free boundary problem arising from the kinetic assumption

$$v_n = f. \tag{4}$$

The main difficulty herein stems from the nonlocal coupling of the driving force to the elliptic problem of calculating the displacement. My first approach to an analysis uses an approximate elastic energy for a phase boundary with small slope; the second treats the general problem by considering the evolution of sets of finite perimeter.

Small slope approximation. Assuming that the phase boundary can be described by the graph of a shallow function g with periodic boundary conditions, one can formally approximate the model. The resulting problem is given in Fourier space by the equation

$$\hat{g}_t(k) = -|k|\,\hat{g}(k) + \hat{\varphi}(k) + \hat{F}(k). \tag{5}$$

Here, the effect of the precipitates and that of an applied stress on the driving force are collected into the local forcing $\varphi = \varphi(x, g(x))$ and a constant external load F.

We have proven existence of a solution to this problem, existence of a threshold force F^* up to which there is a stationary solution to the problem and existence of time-space periodic solutions for $F > F^*$. The physical implication of this is that the phase boundary is stuck up to a critical applied force and moves freely with a macroscopic average velocity thereafter.

The general proof of existence of a solution to the equation uses semigroup methods. In order to assert the existence of a threshold force and that of a time-space periodic solution, we use the Schauder fixed point theorem together with compact embeddings of fractional Sobolev spaces. The latter work follows [1], where the reaction-diffusion equation is considered with $|k|$ replaced by $|k|^2$. However, in our case, one cannot use elliptic or parabolic regularity.

In current work, we are examining the depinning transition of these interfaces both numerically and analytically. A critical power law behavior for the average velocity of the interface can be seen in simulations.

The general problem. For the full model, we have proven the existence of a solution on a bounded domain Ω for non-zero surface energy. We rely on an implicit time discretization for a set evolution model as employed in [2] for a purely curvature driven interface. The main difficulty here lies in the nonlocality of the problem due to the coupling with the elliptic equation, since it is necessary to obtain uniform bounds on the L^∞ norm of the forcing.

Given an initial condition, we build a piecewise constant approximation of the evolving set $E(t)$ (and thus of the evolving phase boundary) by minimizing the set function

$$\mathcal{F}^h(E, E_0) = \mathcal{F}_{\text{elastic}}(E) + c\int_\Omega |\nabla \chi_E| + \frac{1}{h}\int_{E \triangle E_0} \operatorname{dist}(x, \partial E_0)\,\mathrm{d}x \tag{6}$$

at each timestep of duration h. The first term in this energy is the already familiar elastic energy. The second term is equal to the surface energy term introduced before, written now as the variation of a characteristic function. The third term—an integral over the symmetric set difference $E \triangle E_0$—is chosen such that its variation produces a discretized normal velocity of the interface.

For given $h > 0$ and E_0 of finite perimeter, existence of a minimizer follows from the boundedness of all involved energies and the SBV compactness and closedness theorems. One must now establish convergence as $h \to 0$ of the piecewise constant approximation $\chi_{E(t)}$ to a function

$$X \colon \Omega \times [0, T] \longrightarrow \{0, 1\}, \tag{7}$$

which requires strong convergence of the family of characteristic functions. To this end, we introduce a further regularization of the elastic energy $\mathcal{F}^{\varepsilon}_{\text{elastic}}$ through mollification of the transformation strain. We then have $\mathcal{F}^{\varepsilon,h} \xrightarrow{\Gamma} \mathcal{F}^{h}$ and the piecewise constant approximation obtained from sequentially minimizing $\mathcal{F}^{\varepsilon,h}$, for $\varepsilon = h^{1/n}$, converges strongly as $h \to 0$. For a uniformly smooth phase boundary, the resulting normal velocity equals the one in (4).

Current work focuses on numerics and establishing an existence result for time-space periodic solutions. The nature of pinned solutions under a finite applied stress which comprise local energy minima is also being examined.

References

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Reporter: Patrick W. Dondl

Participants

Dr. Stefan Adams
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Dr. Marek Biskup
Department of Mathematics
UCLA
405, Hilgard Ave.
Los Angeles , CA 90095-1555
USA

Dr. Xavier Blanc
Universite Pierre et Marie Curie
Laboratoire Jacques-Louis Lions
Boite courrier 187
4 place Jussieu
F-75252 Paris Cedex 05

Prof. Dr. Isabelle Catto
CEREMADE
Universite Paris Dauphine
Place du Marechal de Lattre de
Tassigny
F-75775 Paris Cedex 16

Dr. Isaac Vikram Chenchiah
Department of Mathematics
University of Bristol
University Walk
GB-Bristol , BS8 1TW

Dr. Nicolas Dirr
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Patrick W. Dondl
Applied and Computational Mathematics
MSC 104-44
California Institute of Technology
Pasadena , CA 91125
USA

Prof. Dr. Dirk Hundertmark
School of Maths and Statistics
The University of Birmingham
Edgbaston
GB-Birmingham , B15 2TT

Prof. Dr. Frederic Klopp
Departement de Mathematiques
Institut Galilee
Universite Paris XIII
99 Av. J.-B. Clement
F-93430 Villetaneuse

Prof. Dr. Wolfgang König
Mathematisches Institut
Universität Leipzig
Johannisgasse 26
04103 Leipzig

Prof. Claude Le Bris
CERMICS - ENPC
Cite Descartes, Champs-sur-Marne
6 et 8 avenue Blaise Pascal
F-77455 Marne La Vallee Cedex 2

Dr. Mathieu Lewin
Departement de Mathematiques
Universite de Cergy-Pontoise
Site Saint-Martin, BP 222
2, avenue Adolphe Chauvin
F-95302 Cergy-Pontoise Cedex

Dr. Robert Sims
Department of Mathematics
University of California, Davis
1, Shields Avenue
Davis , CA 95616-8633
USA

Prof. Dr. Valery P. Smyshlyaev
Department of Mathematical Sciences
University of Bath
Claverton Down
GB-Bath BA2 7AY

Prof. Dr. Jan Philip Solovej
Institut for Matematiske Fag
Kobenhavns Universitet
Universitetsparken 5
DK-2100 Kobenhavn

Dr. Ivan Veselic
Fakultät für Mathematik
TU Chemnitz
Reichenhainer Str. 41
09126 Chemnitz

Prof. Dr. Stephen J. Watson
Department of Mathematics
University of Glasgow
University Gardens
GB-Glasgow , G12 8QW

Dr. Johannes Zimmer
Department of Mathematical Sciences
University of Bath
GB-Bath BA2 7AY