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# SPACE-TIME COMPLEXITY IN SOLID STATE MODELS

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## 1. Introduction

In this Workshop on symmetry-breaking it is appropriate to include the evolving fields of nonlinear-nonequilibrium systems in which transitions to and between various degrees of "complexity" (including "chaos") occur in time or space or both. These notions naturally bring together phenomena of pattern formation and chaos and therefore have ramifications for a huge array of natural sciences [1,2] -- astrophysics, plasmas and lasers, hydrodynamics, field theory, materials and solid state theory, optics and electronics, biology, pattern recognition and evolution, etc. Our particular concerns here are with examples from solid state and condensed matter.

We emphasize three general points: (1) As has been said about many-body physics, "more is different" -- not just quantitatively but qualitatively. This is equally true of the subject of chaos. The elegant developments [3] of recent years understanding classes of one-dimensional maps is extremely important, motivating as it does hopes of "universal" scenarios for transitions to chaos. However, much remains to be understood -- e.g., how to characterize the qualities of the chaos itself and how to incorporate realistic many-degree-of-freedom systems into low-dimensional maps scenarios. One response has been to merge the complementary faces of strongly coherent ("soliton-like") space-time structures with intrinsically incoherent chaotic notions [1,2]; (2) The last remark leads directly to the observation that spatial pattern formation (as a typical quiescent precursor to chaos) and low-dimensional chaos are frequently intimately related, with strong remnants of the coherent structures

persisting in the chaotic regime and the associated collective coordinates providing (at least conceptually) a basis for mode reduction. We frequently refer to "self-organization" and to "coexisting coherence and chaos" and these are usually important to transport and predictability. Complexity in space-time is an appropriate concept also because it is becoming increasingly clear (see below) that space and time should be placed on a common footing and partial differential equations, cellular automata and coupled map lattices viewed in a unified manner. In particular, mappings to higher dimensional equilibrium (Hamiltonian) systems with competing interactions (leading to inhomogeneous ground states, i.e. long-time attractors) appear to be a unifying key [2]; (3) Finally, we emphasize our belief that condensed matter materials, and models thereof, will play an increasingly central role in studies of space-time complexity -- because of the great variety of laboratory scale, highly controlled materials which are available. There is of course direct practical importance for, e.g., device performance, but these are also accessible stepping stones to probing far more general issues of space-time complexity. Imaginative experimental designs in the condensed matter field are now expanding rapidly in number [4]. Of special interest is the availability of controlled, reproducible reduced-dimensional materials -- e.g. polymers, quasi-one and two-dimensional materials, layered compounds, surface structures, artifically structure materials (e.g. by molecular beam epitaxy). Such real systems provide the basis for probing true space-time competition but without yet facing full three-dimensional turbulence.

Our own recent concerns with solid state models exhibiting space-time complexity have focused on three separate kinds of contexts. First, we may consider purely structural disorder in classical equilibrium Hamiltonian systems with competing (incommensurate) interactions or periods (the analogue of purely temporal problems with two or more incommensurate frequencies). Such competitions are now appreciated to occur in a large variety of solid state materials. They are responsible for

ground states and free energy minima which are spatially inhomogeneous. Very familiar experimentally-observed examples are [5] commensurate-incommensurate phase transitions where the incommensurate phase is a distribution of kink- or domain-wall-like "discommensurations," which may be regularly distributed in a superlattice or locally-pinned (e.g. by lattice discreteness) in an irregular ("chaotic") metastable configuration. Much is now known, both experimentally and theoretically, about such "frustration" problems but much remains to understand -- particularly, large amplitude dynamics or the introduction of several competing length scales (see section 2).

Second, we have examined [1,2] a range of classical space-time dependent systems corresponding to nonlinear partial differential equations (p.d.e.s) or coupled systems of large numbers of nonlinear ordinary differential equations. Since much of condensed matter modeling is built around nonlinear oscillators, we have concentrated on systems such as driven, damped (i.e. non-Hamiltonian) sine-Gordon equations with various boundary conditions and in one and two dimensions. These are representative of many quasi-one- and two-dimensional materials [1,2]. Such studies fit into the growing field of perturbed p.d.e.s motivated by many different physical problems [1-4,6]. It is increasingly appreciated that there are typical ways that space-time complexity (attractors such as space-time intermittency) is manifested. This begins to unify behavior not only in classes of p.d.e.s, but also cellular automata and coupled map lattices [1,2]. We have reviewed results on classical space-time complex systems elsewhere [1,2]. Here we recall only two general lessons: (i) both localized (~ "solitons") and extended (~ "radiation") modes almost are always involved in the transition to chaos and the chaotic evolution; and (ii) synergetic mappings are now becoming apparent between p.d.e.s and cellular automata and higher-dimension equilibrium Hamiltonians [2,7]. The effective Hamiltonians exhibit competing interactions and this provides the conceptual basis for "inhomogeneous" space-time attractors as in the purely spatial chaos mentioned above.

Third, solid-state physics can provide [8] some interesting new quantum Hamiltonian models with which to study the poorly understood concept of "quantum chaos", i.e. quantum and semi-classical behavior in integrable and nonintegrable quantum Hamiltonians (see section 3).

## 2. A Model with Three Competing Lengths

The simplest description of incommensurate solid state the structures is based on a one-dimensional Frenkel-Kontorova model with free energy [5,9]

$$F = \sum_{i=1}^{N} \{V(U_i) + W(U_{i+1}-U_i) - \mu(U_N-U_0\} \quad , \tag{1}$$

where W is the nearest-neighbor interaction potential between particles each of which moves in a nonlinear local potential V, e.g. $V(U) = \cos U$. $\{U_i\}$ are, e.g., displacements and $\mu$ is a chemical potential. Usually W is taken to be a harmonic spring, e.g. $W = (U_{i+1}-U_i-\ell)^2$, with equilibrium lattice constant $\ell$. There are a number of variations on this basic model which may be important. One is to include non-convex interparticle interactions, which can arise from, e.g., RKKY magnetic couplings. To be specific we consider [10] an extreme Ising-like form for W:

$$U_{i+1} - U_i = \ell_1 \text{ or } \ell_2. \tag{2}$$

In model (1) with harmonic springs there can be only two incommensurate lengths, $\ell$ and $2\pi$. However, with the modification (2), $\ell_1$, $\ell_2$ and $2\pi$ may all three be incommensurate.

It has been possible to investigate the mean-field states of the general model (1) and (2) analytically and numerically and the results are surprisingly complicated [10]. To summarize: (i) Typically, we find many intermediate phases as we vary $\mu$. This is in contrast to results where a uniform lattice constant is imposed, which predicts a first order transition; (ii) The average separation between phases forms a partial "devil's staircase" [9]; (iii) Most surprisingly, the plateaux

of the staircase occur at certain incommensurate concentrations characterized by the three lengths, and all of the incommensurate configurations are locked; (iv) The locations of most of the plateaux can be predicted on the basis of a circle map (below); (v) If both $\ell_1$ and $\ell_2$ are rational with respect to the $2\pi$ periodicity of V(U), then a finite number of transitions occur, all of which are first order. We now briefly describe some of these features.

A direct (but non-trivial) evaluation of the minimum energy states provided key input for a constructive theory (see Ref. (10)). This will be illustrated with $\ell_1$ and $\ell_2$ taking the specific values $(\sqrt{3.5} + \sqrt{5} - \sqrt{2} - 2)\pi$ and $\pi\sqrt{3.5}$, respectively. In Fig. 1 we show the (free) energy per particle $F_M^N/N$ versus the "configuration magnetization" $M(0 \leq M \leq N)$, with $M = \Sigma\, \sigma_n$ and $\sigma_n = 0$ or 1 for $U_{n+1}-U_n = \ell_1$ or $\ell_2$, respectively. Adding a finite chemical potential term $\mu(U_N-U_0) = \mu M$ simply tilts the whole function F. Note that $F_M$ is (at least very close numerically) continuous, convex, and has several most prominent sharp corners. The locations $c(\equiv M/N)$ as a function of $\mu$ are shown in Fig. 2 ($N = 5 \times 10^3$). Note that the mean lattice constant $\ell = (1-c)\ell_1 + c\ell_2$. We observe a typical partial devil's staircase and the magnification [10] suggests near completeness in some regions. Since $\tilde{c}(\mu)$ ($\tilde{c} \equiv 1-c$) appears to increase monotonically, this supports the convexity of $F_M$. For each state (step) we can calculate the integrated probability D(v) to find a particle between 0 and v ($< 2\pi$) with $D(v) = N^{-1} \Sigma\, \theta(v-U_i \bmod 2\pi)$. D(v) is shown in Fig. 3 for the configurations $\{U_i\}$ corresponding to the corner of $F_M^N$ (i.e. plateau of $\tilde{c}(\mu)$) at $M = 253$ (i.e. $\tilde{c} = 0.832$). Note that the $U_i$ are distributed in a finite number of bands (the non-horizontal lines in the figure) to which particles are restricted. Furthermore the particle density within the bands is uniform. These are the primary observations which permit an analysis [10] based on a transformation from the linear map, $T(x) = x + \ell_1$ or $\ell_2 \bmod 2\pi$, to a so-called "one-circle band structure".

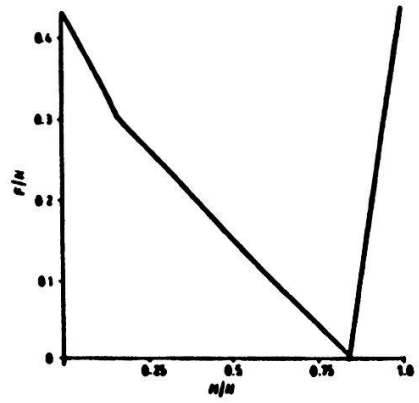

Fig. 1 Free energy per particle F/N versus mean magnetization M/N or concentration $\tilde{c}$, for chemical potential $\mu = 0$. (After Ref. (10).

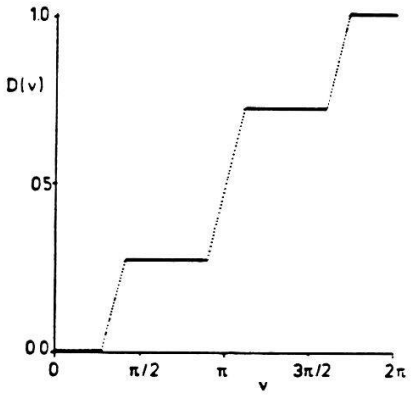


Fig. 3: Integrated particle density D(ν) (see text) for a 3-band configuration.

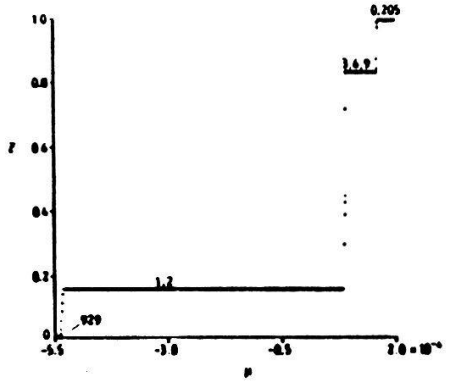

Fig. 2 Minimizing concentration $\tilde{c}$ of $F^M$ versus $\mu$. Steps are labeled by allowed p values (see text) in range (-2,000, 2,000).

The one-circle band structure analysis shows [10] that the minimum energy configurations should be characterized by a set of just <u>four</u> integers p, q, r, s, and this is confirmed numerically. These numbers determine the total width of the bands and mean lattice spacings. The plateaux widths depend in detail on the form of V(U). For each set of integers p, q, r, s satisfying certain topological constraints there exists a one-circle band structure and vice-versa, and the corresponding configurations are <u>incommensurate</u> with explicit form $U_i - U_0 = f(i\omega + \beta) - f(\beta)$, where $f(x) = x(\ell_1 - s\delta)/\omega + xp\delta/2\pi + g(x)$, $g(x)$ is $2\pi$-periodic, $\delta = \ell_2 - \ell_1$, and $\beta$ is an initial phase. The wavevector of the modulation is $\omega = 2\pi(\ell_1 + 2\pi r - s\delta)/(2\pi q - p\delta)$, and the concentration of lattice constants $\ell_2$ is $c(p) = [p\ell_1 - 2\pi \ \mathrm{Int}(p\ell_1/2\pi)] /(2\pi q - p\delta)$ with $q = \mathrm{Int}(p\delta/2\pi) + 1$. Note that there can be several possible wavevectors (which depends on r

and s as well as p) for a single configuration labeled by p since the mean lattice constant only depends on p: see Ref. (10) for several examples.

## 3. A Quantum Chaos Model

We briefly summarize recent results obtained for the following 3-spin model [8,11]:

$$H = J \sum_{i=1}^{3} \{\vec{S}_i \cdot \vec{S}_{i+1} + \sigma S_i^z S_{i+1}^z\} \quad . \tag{3}$$

Here $J > 0$, $-1 \leq \sigma \leq 0$ and boundary conditions are periodic. Thus we have a triangle with antiferromagnetic coupling and easy-plane symmetry for $\sigma < 0$. The interest in this and similar models is that we can easily control both "quantumness" $\hbar(\hbar \sim S^{-1})$, and integrability, because (3) is integrable for $\sigma = 0$ but increasingly nonintegrable as $\sigma$ decreases from 0. We have used these controls to study quantum irregular spectra [8], and associated wavefunctions [11], as functions of both nonintegrability and quantumness. In this way we numerically identified: (i) scaling in the statistical averages of second-order differences of eigenvalues (i.e. curvatures of $E(\sigma)$) as $S \to \infty$ (i.e. the semiclassical regime); (ii) quasi-fractal features in the level distribution for irregular spectra; and (iii) so called "fat fractal" [12] properties discriminating wave-functions in regular and irregular regimes.

Since our aim is to understand semiclassical ($S \gg 1$) analogues of classically chaotic and nonchaotic regimes, we briefly summarize the classical results. (Of course, there is a possibility that the classical limit $S = \infty$ is a singular point.) Model (3) is in fact very interesting classically in its own right: for $\sigma \neq 0$ it presents a 4-dimensional phase space and, by varying $\sigma$ and energy E, a systematic study of Arnol'd diffusion will be possible. Because the coupling is antiferromagnetic, complex ("chaotic") dynamics occurs at low energies and the frustration is overcome at high energies. Specifically, studies of Poincaré surface sections and power spectra show [8]

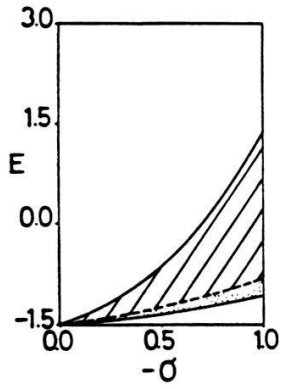


Fig. 4: Schematic variation of classically regular and chaotic regions as E and σ are varied. Hatched and speckled regions correspond, respectively, to "global" and "localized" chaos. Remaining regions contain dominantly regular orbits.

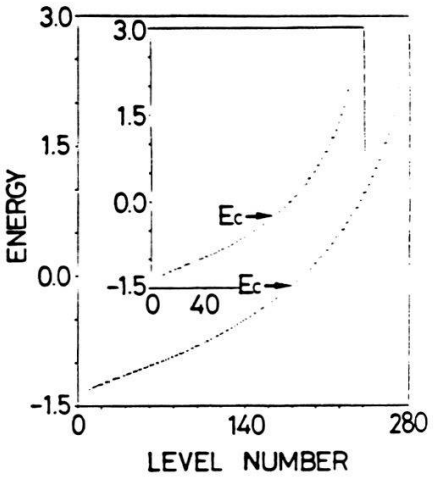


Fig. 5: Quantum energy levels for S = 22½ and 16½ (insert) with σ = -0.3. See Ref. (8) for details.

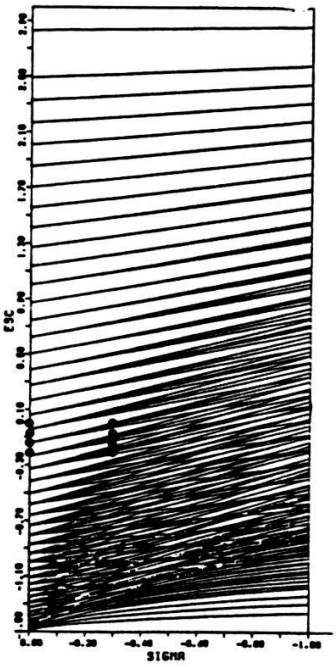

Fig. 6: σ-dependent quantum energy levels for S = 16½ with $\tilde{E} = E/S(S + 1)$. Fractal diagnostics for the regions indicated are reported in Ref. (11).

that at low energies near the ground state $E_G = -1.5J$ the phase space is dominated by regular orbits corresponding to spin waves. With increasing energy the phase space is still restricted but there are some "ergodic" K.A.M. trajectories, i.e., irregular orbits in bounded regions of phase space. Above a lower "transition energy" diffusion through all phase space occurs and there is "global" chaos. Above an upper "critical"

energy region, orbits again become regular K.A.M. This senario [8] is summarized schematically in Fig. (4).

We now ask whether quantum analogues of these various regimes can be identified. Dynamic quantum properties are presently under investigation -- for example the quantum propagator and the energy-dependent diffusion coefficient. Because of the (numerical) control of both S and $\sigma$, it has already been possible to discover new features in the static properties of eigenlevel distributions and associated wavefunctions. We briefly mention three properties.

First, the energy level distribution itself, for large S, already shows [8] evidence of the classically chaotic regimes. In particular (see Fig. (5)), a "critical" or "crossover" energy $E_c(\sigma)$ is evident: for $E \lesssim E_c$, energy levels are irregularly distributed, whereas for $E \gtrsim E_c$ steps of well-separated clustered levels dominate. It is natural to associate the structure for $E \gtrsim E_c$ with quantized periodic orbits. The coexistence of band-like and localized energy level regions for $\sigma < 0$ is somewhat reminiscent of Anderson localization [13]. The essential ingredient involved in quantum irregular spectra is the avoided crossing (repulsion) of nearby levels -- see Fig. (6).

Motivated by Fig. (6) and by the success of scaling theories in Anderson localization [13], we have examined [8] as our second criterion the local curvatures of the $\sigma$-dependent energy eigenvalues, viz.

$$\Delta^2 E/\Delta\sigma^2 \equiv [E(\sigma + \Delta\sigma) - 2E(\sigma) + E(\sigma - \Delta\sigma)]/(\Delta\sigma)^2 \quad . \qquad (4)$$

This assesses a sensitivity of eigenvalues to the nonintegrability parameter. Convergence was obtained with $\Delta\sigma = 5 \times 10^{-4}$ and statistics were improved by averaging over similar energy ranges (c.f. Figs. (4-6)). The statistical averages grow with increasing S below a critical ($\sigma$-dependent) energy (the quantum analog of $E_c$) but are essentially independent of S above this energy. The characteristic trends for large S are most evident in terms of the dimensionless standard deviation

$$g(S) \equiv \langle(\Delta^2 E/\Delta\sigma^2 - \langle\Delta^2 E/\Delta\sigma^2\rangle)^2\rangle^{1/2}/\langle\Delta^2 E/\Delta\sigma^2\rangle \quad , \qquad (5)$$

where averages $\langle\cdots\rangle$ are taken in appropriate energy ranges. We have found [8] strong numerical evidence for a large S scaling behavior:

$$g(\Lambda S/g(S) = \Lambda^{\beta(\sigma)} \quad . \qquad (6)$$

Strikingly, the exponent $\beta(\sigma)$ is > 0 in irregular regions of the energy level distribution and < 0 in the regular regions, and we have proposed $\beta(\sigma) = 0$ as a promising criterion for the quantum version of classical chaotic-nonchaotic crossovers: neither the irregularity of the spectrum $E(\sigma)$, nor the local curvatures for fixed S provides an adequate criterion.

It is tempting to think of Fig. (6) and result (6) in terms of "fractals" [3]. One might imagine a successive similarity of the energy level structure (as a function of $\sigma$) on smaller scales (> $\hbar$) as S is increased. In fact our third criterion has focused on the associated wave function structure. We have found [11] that projected binary patterns of wavefunctions exhibit a self-similar scaling property for large S, whose exponent and variation for increasing S appear to connect the classical chaos with a quantum analogue in a natural way -- the semiclassical wavefunctions vividly display their integrable or nonintegrable nature. Technically, true fractal behavior does not obtain, but rather so-called "fat fractal" scaling recently proposed [12] for low-dimensional classical maps with chaotic phase space orbits punctured by holes of K.A.M. or periodic orbits.

## 4. Summary

We have advocated our belief [1,2] that complexity (the symmetry-breaking transitions and the complexities, including chaos, themselves) in spacetime represents the new, and in many respects accessible, frontier for dynamical systems research, succeeding the exciting systematics discovered for low-dimensional maps [3]. Many elements of analysis are involved in this nonlinear-nonequilibrium field from applied mathematics and

theoretical modeling to large-scale and dedicated computing and cellular automata to imaginative experiments. Likewise, the physical applications occur in essentially every scientific discipline from biology to astrophysics. Here, we have emphasized [4] the growing importance of condensed matter and materials science, which can provide bench-top experiments and the possibility of real systems in reduced dimensions.

We are indebted to discussions and collaborations with several colleagues, especially S. Aubry, K. Fesser, and K. Nakamura.

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