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 "complex-
ity" (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 evolu-
tion, 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 quanti-
tatively but qualitatively. This is equally true of the subject
of chaos. The elegant developments [3] of recent years under-
standing classes of one-dimensional maps is extremely important,
motivating as it does hopes of "universal" scenarios for transi-
tions 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 inhomo-
geneous. Very familiar experimentally-observed examples are [5]
commensurate-incommensurate phase transitions where the incom-
mensurate 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 "frus-
tration" problems but much remains to understand -- particu-
larly, 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 dif-
ferential equations (p.d.e.s) or coupled systems of large num-
bers of nonlinear ordinary differential equations. Since much
of condensed matter modeling is built around nonlinear oscilla-
tors, 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 intermit-
tency) 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 transi-
tion 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 μ 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 ℓ. There are a number of variations on this basic model which may be important. One is to include non-convex interparticle inter-actions, 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 incom-mensurate lengths, ℓ and 2π. However, with the modification (2), ℓ_1, ℓ_2 and 2π 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 sum-marize: (i) Typically, we find many intermediate phases as we vary μ. 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 <u>incommensurate</u> concentrations characterized by the three lengths, and all of the incommensurate configurations are <u>locked</u>; (iv) The locations of most of the plateaux can be predicted on the basis of a circle map (below); (v) If both ℓ_1 and ℓ_2 are rational with respect to the 2π 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 ℓ_1 and ℓ_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 ℓ_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 μ 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 $D(v) = N^{-1} \Sigma \theta(v-U_i$ mod 2π). $D(v)$ 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 <u>bands</u> (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 ℓ_2 mod 2π, to a so-called "one-circle band structure".
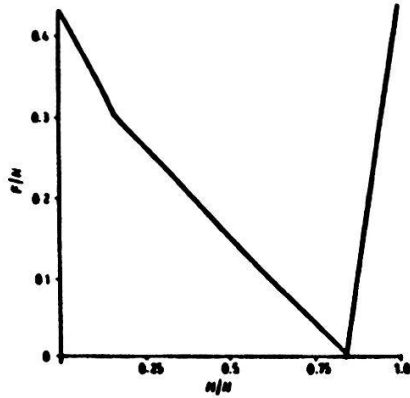
Fig. 1 Free energy per parti-
cle F/N versus mean magnetiza-
tion M/N or concentration $\tilde{c}$,
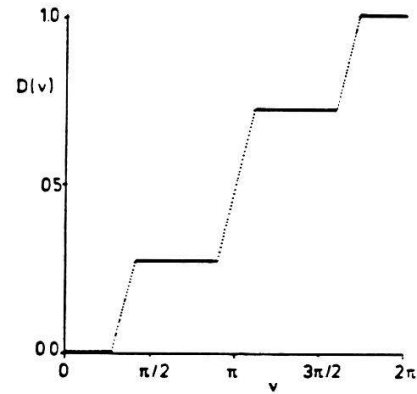for chemical potential $\mu = 0$.
(After Ref. (10).

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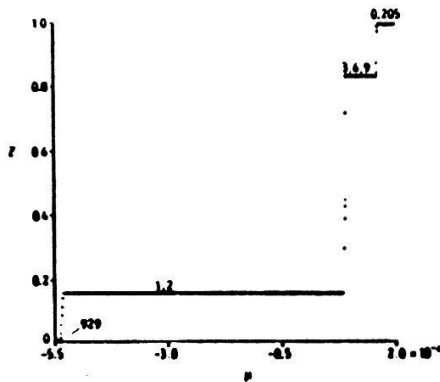3-band configuration.

Fig. 2 Minimizing concentration $\tilde{c}$ of
F^M versus μ. 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 char-
acterized by a set of just <u>four</u>
integers p, q, r, s, and this is con-
firmed 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 2π-periodic, $\delta = \ell_2 - \ell_1$, and β is an initial phase. The wave-
vector 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 ℓ_2 is $c(p) = [p\ell_1 -$
2π $Int(p\ell_1/2\pi)]$ $/(2\pi q - p\delta)$ with $q = Int(p\delta/2\pi) + 1$. 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 σ decreases from 0. We have used
these controls to study quantum irregular spectra [8], and
associated wavefunctions [11], as functions of both nonintegra-
bility and quantumness. In this way we numerically identified:
(i) scaling in the statistical averages of second-order differ-
ences 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 ($S \gg 1$) ana-
logues of classically chaotic and nonchaotic regimes, we briefly
summarize the classical results. (Of course, there is a possi-
bility 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 σ and energy E, a systematic study of Arnol'd diffu-
sion will be possible. Because the coupling is antiferromag-
netic, complex ("chaotic") dynamics occurs at low energies and
the frustration is overcome at high energies. Specifically,
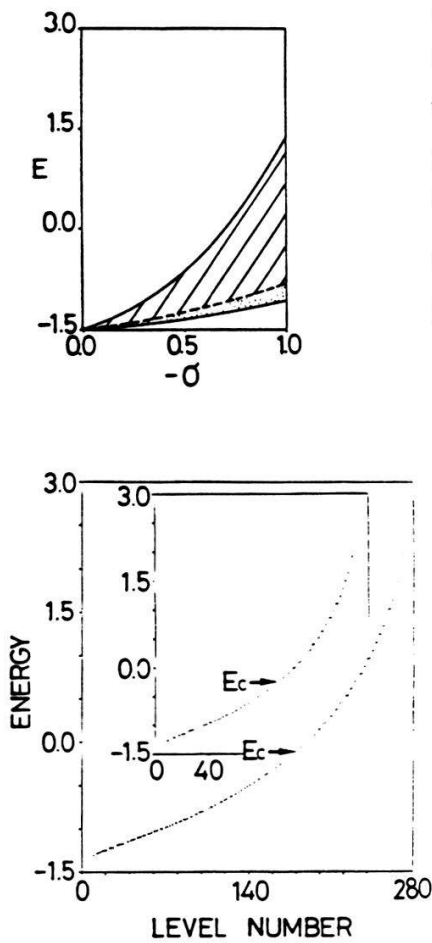studies of Poincaré surface sections and power spectra show [8]

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.
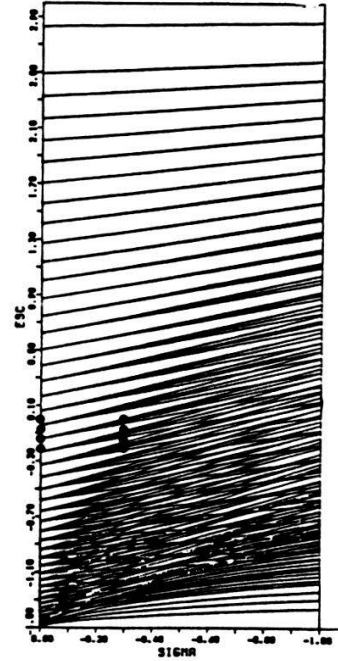

Fig. 5: Quantum energy levels for S = 22½ and 16½ (insert) with σ = -0.3. See Ref. (8) for details.

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. Be-
cause of the (numerical) control of both S and σ, 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 co-
existence of band-like and localized energy level regions for
σ < 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 σ-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 nonintegra-
bility 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 (σ-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

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

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

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

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 σ) 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.

4. References

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