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MASTER

PHYSICS IN FEW DIMENSIONS

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Physics in Few Dimensions

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This article is a qualitative account of some aspects of physics in few dimensions, and its relationship to nonlinear field theories. After a survey of materials and some of the models that have been used to describe them, the various methods of solution are compared and contrasted. The roles of exact results, operator representations and the renormalization group transformation are described, and a uniform picture of the behavior of low-dimensional systems is presented.

I. INTRODUCTION

Many of the fundamental problems of condensed matter physics may be regarded as examples of nonlinear field theories. This point of view has been advantageous for the quantum-mechanical many-body problem and for the modern theory of phase transitions, leading to successful theories of single-particle and collective phenomena in a wide variety of physical systems. It is the basis for our current understanding of superconductivity and superfluidity, and has led to a deeper understanding of the universal cooperative effects which are observed in the neighborhood of a critical point. Most of these developments have relied upon the techniques of quantum field theory, and have made little reference to concepts that have arisen in a purely classical context. More recently, however, this situation has changed, and some of the approaches to physics in one and two space dimensions have been much closer in spirit to the ideas of classical nonlinear field theory; references to the sine-Gordon equation, solitons, breathers, inverse scattering, etc., have become relatively commonplace in the literature of elementary particle and condensed matter physics.

A feeling for the relevance of these concepts and their supplementary relationship to the more "conventional" approach may be obtained by considering several examples from condensed matter physics. In what follows, there will be no reference to the theory of non-integrable systems, although its influence is beginning to make itself felt, for example, in attempts to understand some aspects of the theory of incommensurate structures[1].

The systems of interest are quite diverse in their physical characteristics. Some are quantum mechanical and one dimensional, others are classical and two dimensional. But it turns out that there is a common thread to their mathematical formulation: a remarkably large number of models are equivalent to each other, either exactly or in the asymptotic properties which govern the kinds of long-ranged order that might be established. All bear some relationship to the sine-Gordon equation.

The impetus for these developments has come from both theory and experiment, from the desire for a unified view of two-dimensional models as well

as a need to understand a number of unusual observations. The ingenuity of the synthetic chemist and the experimental physicist has been a continual driving force in the whole field, and it is appropriate to start out with some brief mention of the materials they have investigated, before going on to describe the mathematical models, and the methods that have been devised in order to solve them.

II. MATERIALS

Low-dimensional behavior arises in two principal ways. Some materials are extremely anisotropic, consisting of atoms, molecules or ions arranged in chains or in layers, which are weakly coupled to their environment, and act independently over a wide range of temperatures. The structure imposes its own constraints on the motion of electrons, and this leads to characteristic low-dimensional behavior of the electrical properties. The alternative is to have a restrictive geometry; a free film or a film adsorbed on a surface are essentially two dimensional, whereas particles confined to narrow channels may have a one dimensional character. In most cases there are circumstances in which the true three-dimensional nature of the system makes itself felt, and understanding the crossover to this regime is part of the interest in the problem. The purpose of studying these systems is to look for phenomena that may not occur, or may be difficult to produce in more isotropic materials: effects of disorder are expected to be more pronounced, and certain kinds of phase transition may take place more readily. It has long been a hope to find superconductivity at relatively high temperatures in anisotropic organic materials, where strong electron-electron interactions may be produced by an excitonic mechanism[2].

All of these effects are likely to involve an interplay between the many degrees of freedom which reside in a molecular crystal--the spin and translation of electrons or the spin, orientation, vibration and translation of the molecules. For this reason, it is often quite difficult to extract, from rather indirect experimental information, the primary mechanism which drives the behavior of a particular physical system. The common approach has been to solve a number of simplified models, in order to discover the particular effects to look out for and to limit the possible range of explanations of a given experiment.

A few examples will illustrate the nature of the systems which have been investigated. One-dimensional materials frequently contain rather flat organic molecules[3] such as TTF (tetrathiafulvalene), TSeF (tetraselenofulvalene), TCNQ (tetracyanoquinoodimethane) and TMTSF (tetramethyltetraselenofulvalene), all of which may be arranged in closely packed stacks. In TTFCuBDT, long-ranged correlations in chains of localized spins conspire with peculiarities of the lattice vibrations to produce a dimerized state[4] (spin-Peierls transition). The organic metals TTF-TCNQ, TSeF-TCNQ and $(TMTSF)_2PF_6$ are electrical conductors because charge transfer from donor to acceptor molecules leaves a partially filled band of states[3]. The conductivity of these systems increases to a quite high value as the temperature is lowered, but ultimately this is reversed by a metal-insulator transition. However, at sufficiently high pressure, $(TMTSF)_2PF_6$ becomes a superconductor. An example of a so-called molecular metal is $Hg_{3-\delta}AsF_6$, which consists of chains of Hg ions arranged in planes and interspersed with AsF_6^- ions. Its peculiar properties are a consequence of the lack of commensurability between the Hg chains and the AsF_6^- lattice (δ is a function of temperature and is about 0.2) At room temperature, the weakly coupled Hg chains form one-dimensional liquids[5], but they freeze at about 120 K. This transition is unusual in that it is an example of continuous freezing. At much lower temperatures the material becomes a superconductor[6], but the origin and properties of this state are not fully understood. An entire session of this conference is concerned with the properties of polyacetylene, a linear system which is thought to form a dimerized chain with soliton dislocations.

Much of the recent interest in two-dimensional materials has been centered upon a class of systems which have a phase transition but are unable to establish the related long-ranged order because of the destructive effect of thermal fluctuations. They accomplish this as the temperature is decreased below a certain value, by remaining on the verge of a transition to an ordered state: every point is critical. Solids, superconductors, superfluids and some phases of liquid crystals are expected to have this behavior in two dimensions, and verification has been sought in adsorbed layers or freely-suspended films. Another interesting property of overlayers is the existence of periodic structures that may be commensurate or incommensurate with the substrate lattice. This problem has been investigated by the scattering of neutrons, x-rays and electrons as well as by photoemission experiments, and, although a picture of what is going on has steadily been developed, it is still far from complete. Other two-dimensional forms of spin ordering, displacive phase transitions and charge-density wave states are to be found in bulk materials with a layered structure. A more extensive review of this whole subject may be found in the proceedings of the 1979 Kyoto summer school[7] and the 1980 Lake Geneva, Wisconsin conference[8].

III. MODELS

At first sight it seems inappropriate to pay so much attention to cyrstalline solids and lattice models in a discussion of nonlinear field theories, but there is much to be gained from relating one to the other by taking the continuum limit.

The location of a point in a simple cubic lattice is specified by a vector $\vec{r} = s\vec{n}$, where $\vec{n}$ has integer components and s is the lattice spacing. Correlation functions have a characteristic length scale $s\xi$, where ξ, the coherence length of the lattice model, is a pure number. A field theory is obtained by taking the continuum limit $s \to 0$, in which finite differences become derivatives, and lattice sums become integrals. The advantage of considering this limit, which is clearly ficticious for a real solid, is that it focuses attention on the asymptotic properties of correlation functions, and forces us to consider behavior at a critical point. For if the length scale $s\xi$, and position vector $\vec{r}$ are to remain finite as $s \to 0$, it is necessary that $\xi \to \infty$ (which is the case at a critical point) and $|\vec{n}| \to \infty$ (which is the asymptotic limit). Equally, the continuum limit is useful for a field theory when the critical properties of the corresponding lattice model are known.

In the present context, however, there is a further important reason for taking the continuum limit--it is crucial for establishing the relationship between models and obtaining a unified picture of physics in two dimensions. Space does not permit an account of the technical developments necessary fc the implementation of this program, but a survey of some of the inte_sting Hamiltonians should give at least some idea of the kinds of system under consideration. Classical, two-dimensional models will be described first.

Potts Models[9]

$$H_p = -J \sum_{n.n.} \delta_{S_i S_j} \qquad (1)$$

with $S_i = 1,2,\ldots q$. Here, the summation is carried over near-neighbor sites i,j on a square lattice. The state of lowest energy has all spins equal and is q-fold degenerate. This Hamiltonian is relevant for adsorbed films[9] and for magnetic systems. (q=2 is identical to the Ising model)

Ashkin-Teller Model[10]

$$H_A = -\sum_{nn} \{J_1 S_i S_j + J_2 T_i T_j + J_3 S_i T_i S_j T_j\} \qquad (2)$$

where $S_i = \pm 1$, $T_i = \pm 1$. This is a two-component lattice gas and, for $J_1 = J_2 = 0$, it is identical to the 4-state Potts model.

Interface Roughening[11]

$$H_R = -\sum_{n,n} f(h_i - h_j) \qquad (3)$$

with $h_i = 0, \pm 1, \pm 2, \ldots$, is a cell model of crystal growth. The constituents are assumed to fill a column of cells to a height h_i at lattice site i. For the physical model, $f(h) = |h|$ (solid-on-solid model), but another case of particular importance is $f(h) = h^2$ (discrete Gaussian model) which is directly related to the Coulomb gas and the xy-model, as will be seen.

Vertex Models[12]

It is imagined that every vertex in a square lattice is connected to its four neighbors by a link, which has a sense (right or left, up or down) specified by an arrow. There are sixteen different kinds of vertex (four links, each with two senses) and each is assigned a different weight. The problem is to sum over all configurations of links. The eight-vertex problem (in which each vertex has an even number of incoming and outgoing arrows) has been solved exactly by Baxter[12]. It is also of interest to consider a more general staggered version of this model with two sets of weights, one for each of two interpenetrating sublattices. Such a model has been shown to be equivalent to the Potts models[13] and to the Ashkin-Teller model[10].

The xy-Model[14]

which has a Hamiltonian given by

$$H_{xy} = -J \sum_{n.n.} \vec{V}_i \cdot \vec{V}_j \qquad (4)$$

where $\vec{V}_i$ is a unit, two-dimensional vector, differs from the preceding models by having a continuous variable at every site. This is clear if $\vec{V}_i \cdot \vec{V}_j$ is rewritten in the form $\cos(\theta_i - \theta_j)$ where θ_i and θ_j are the polar angles of $\vec{V}_i$ and $\vec{V}_j$. This Hamiltonian describes a magnetic system, but it has also been used for the superfluid transition in He^4 films, for which θ_i is the phase of the order parameter. The dual[14] of H_{xy} is a special case of H_R.

Coulomb Gas[14]

$$H_C = -\sum_{all\, i,j} \sum_{Q_i} Q_i Q_j \ln|\vec{r}_i - \vec{r}_j| \qquad (5)$$

Here the summation over i and j extends to all sites (not only near neighbors), and the charges Q_i have values $0, \pm 1, \pm 2, \ldots$. This model is equivalent[14,16] to the discrete Gaussian version of H_R, as mentioned earlier.

It is a remarkable fact that these apparently quite different models are closely related: the partition function of one may be transformed into the partition function of the other, with an appropriate redefinition of parameters. In some cases, the transformation is exact in others it is asymptotically correct for the critical properties[9-16]. It is often possible to find further equivalences between correlation functions. However, the transition to field theory is most directly made via the transformation of all of these models into one-dimensional quantum mechanical systems. The link is provided by the transfer matrix[17] T.

The partition function Z is a sum over all configurations of variables on the lattice. The elements of T consist of the contributions to this sum from pairs of configurations of two neighboring rows of the lattice, and

$$Z = \mathrm{Tr}\, T^N \tag{6}$$

where N is the number of rows. In the thermodynamic limit ($N\to\infty$), Z is dominated by the largest eigenvalue of T. The configurations of a row may also be regarded as states of a one-dimensional quantum system, with T^N playing the role of a transition matrix. In this interpretation, if T is written in the form[18] $\exp(-H)$, then H is the corresponding quantum Hamiltonian, and its ground state gives the largest eigenvalue of T. It may appear that one of the original space dimensions has been lost, but actually it has been replaced by (imaginary) time which, implicitly or explicitly, plays an unavoidable role in quantum mechanics. Following this procedure, every one of the models listed above may be related to the spin Hamiltonian[19]

$$H = H_0 + H_1 + H_2 \tag{7}$$

where

$$H_0 = -\sum_{j=1}^{N}[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y - g\,\sigma_j^z\sigma_{j+1}^z] \tag{8}$$

$$H_1 = \gamma\sum_{j=1}^{N}[\sigma_j^x\sigma_{j+1}^x - \sigma_j^y\sigma_{j+1}^y] \tag{9}$$

and

$$H_2 = -\lambda\sum_{j=1}^{N}(-1)^j[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y - g'\sigma_j^z\sigma_{j+1}^z + h_s\sigma_j^z] \tag{10}$$

Here σ_j^x, σ_j^y and σ_j^z are Pauli matrices. The Hamiltonian H_0 describes the Heisenberg-Ising model, H_1 gives an anisotropy in the xy plane of spin space and H_2 is a dimerization that is related to the staggering of weights in the Baxter model. This is the central model of the field to which all others may be reduced, at least asymptotically[19]. The spin representation (8)-(10) is only one way of writing H. Other useful forms in terms of fermion or boson variables will be introduced later. The parameters, g, γ, λ, g', h_s are known functions of the temperature and the parameters (J, q, etc.) of the original models. It will be seen that H_0 is the critical Hamiltonian while H_1 and H_2 give thermal or field perturbations away from the critical points of the original models.

It is now possible to state how the quantum models, mentioned in Section 2, may be fitted into the picture. The Hamiltonian for a spin-Peierls system[4] is H_0+H_2, where H_0 refers to localized spins in a uniform lattice, and H_2 describes the effects of dimerization in the low-temperature phase. The motion of the mercury ions in $Hg_{3-\delta}AsF_6$, and the spin or charge degrees of freedom of electrons in organic conductors are related to H_0+H_1, but, to show more

explicitly how this comes about, it is necessary to know something about transformations between spins, bosons and fermions. This is described in the next section.

IV. METHODS OF SOLUTION

It is a remarkable feature of one-dimensional physics that, for a number of models, eigenstates and eigenvalues are known exactly. They have been obtained in various equivalent forms--Bethe's ansatz for the wavefunction (see Dr. Andrei's talk), quantum inverse scattering[20] and the semiclassical method for field theory[21]. This whole approach is closely related to the ideas of classical nonlinear physics, and it works for systems which are exactly integrable.

Once an exact solution is available, it might seem that there is little more to be said. However it is not easy to work with the wavefunctions and, with one exception[22], it has not been possible to evaluate correlation functions which are required in order to assess the prospects for various kinds of long-ranged order. Furthermore, the method has not so far succeeded for the most general Hamiltonian of Eqs. (6)-(10), including dimerization, and hence there is every reason to seek alternative approaches, even approximate ones, that are not so specific. Two are of particular importance--operator representations, and the renormalization group method.

The idea of using operator representations is that there are exact relationships between spin, fermion and boson operators, and it may happen that a problem is intractable in one representation but may be exactly soluble in another. Perhaps the best-known example is the Jordan-Wigner transformation[23]

$$\sigma_m^+ = \exp(i\pi \sum_{j=1}^{m-1} c_j^\dagger c_j) c_m^\dagger \tag{11}$$

$$\sigma_m^- = \exp(i\pi \sum_{j=1}^{m-1} c_j^\dagger c_j) c_m \tag{12}$$

where

$$\sigma_m^\pm = 1/2(\sigma_m^x \pm i\sigma_m^y) \tag{13}$$

and c^+_m, c_m are fermion creation and annihilation operators. This transformation is used in solving the two-dimensional Ising model[23], and it may be used for any lattice model. On the other hand the boson representations of spin or fermion operators[24] rely on the continuum limit[25]. For fermions in one dimension, it is possible to distinguish between right-going and left-going particles, with field operators $\psi_+(x)$ and $\psi_-(x)$ respectively. Then $\psi_\pm(x)$ may be written[24]

$$\psi_\pm(x) = \text{const} \exp[-i(\pi/u)^{1/2} \int_{-\infty}^{x} d\xi\, \pi(\xi) \pm i(\pi u)^{1/2} \phi(x)] \tag{14}$$

where $\phi(x)$ is a Bose field and $\pi(x)$ is its conjugate momentum. This transformation is particularly useful, because it is rather easy to evaluate correlation functions when the operators consist of exponentials of Bose fields[24]. Equations (11)-(14) are given in order to show the form of the transformations. More detailed discussions and applications to a number of problems may be found in the literature or in reviews[23,24,25].

The operator representations give the connection between the spin chain and other one dimensional materials, and also show how the sine-Gordon equation comes into the picture. In the continuum limit, the charge- and spin-degrees of freedom of the conduction electrons are decoupled[24], and each may be regarded as a set of spinless fermions which, in turn, are related to $H_0 + H_1$ by a Jordon-Wigner transformation. The Hamiltonian contains products of $\psi_\pm(x)$ and $\psi_\pm^\dagger(x)$ and, introducing the boson representation (14), it is found that the contribution from the integral of $\pi(\xi)$ cancels out leaving a factor proportional to $\cos[(\pi\mu)^{1/2}\phi(x)]$, which is the potential energy density of the sine-Gordon system. Thus, all of these problems, as well as the ordered phase of mercury ions in $Hg_{3-\delta}AsF_6$ (another sine-Gordonn system[5]) are related to the spin chain.

The sine-Gordon equivalence suggests that there may be soliton and breather excitations. However, the fields are quantized and, in contrast to the classical case[21,26], the solution depends on the value of μ. Solitons and breathers exist when μ is less than a critical value, and then the mass of the lowest excitation is a measure of the coherence length in the disordered phase of the corresponding two dimensional problem; since the mass governs the decay in (imaginary) time of a quantum-mechanical system. It is in this region that the sine-Gordon picture contributes most effectively to the solution of this group of problems[24]. If μ is greater than the critical value, there are no solitons and the excitations are massless. This region corresponds to the line of critical points in the two dimensional theories[27], and is more effectively tackled by the renormalization group method.

One way of phrasing the renormalization group method[28] is to focus on some quantity such as the coherence length ξ, and to study the variation of parameters (such as J) required to keep ξs fixed, as s varies. From the resulting flow equations, it is possible to evaluate the critical exponents. Usually this procedure cannot be carried out exactly unless there is a small parameter in which an expansion may be made. It does, however, tell us which are the relevant variables, the ones which must be taken into account in order to get a complete description. The method is most useful in the neighborhood of a fixed point of the transformation, and it is usually necessary to resort to numerical calculations or to some other method of calculation if a more global picture is required. Nevertheless it can be applied in a relatively straightforward way to more complex Hamiltonians, and to include the dimerization H_2, which is quite difficult to deal with otherwise[19].

Clearly, all of these approaches have their advantages and limitations, and it is necessary to resort to a combination of all of them, in order to build up a complete picture of a given problem. The Bethe ansatz or the quantum versions of the inverse scattering method are directly related to classical nonlinear theories. They give exact expressions for the energy spectrum, but it is quite difficult to evaluate correlation functions. The transformations between spins, fermions and bosons may help to turn a problem into a more easily soluble form but, without further help, they do not always give a mass spectrum. They are at their best near a critical point, where the boson form in particular is useful in giving the algebraic decay of correlation functions and expressions for the associated critical exponents[24]. The renormalization group was originally a technique of quantum field theory. It is versatile but does not give a complete analytical solution to a problem if there is no small parameter in which to expand, or if regions far from a fixed point cannot be disregarded.

Nevertheless, by assembling the contributions of all of these techniques, we have come to a unified picture of a large class of one-or two-dimensional

models. The common feature is a line of critical points, along which correlation functions of the classical or quantum models decay algebraically; with exponents that depend upon the position along the line. The boson representations and renormalization group equations lead to relationships between critical exponents in what amounts to an extension of the exact results to problems for which no exact solution exists[19]. Off the critical line, it is necessary to know the mass spectrum or the coherence length and to make use of all of the methods in order to obtain a solution. A survey of this approach and a description of recent work is given in reference 19.

All of these developments have been described in the context of condensed matter physics, but many of the results have been discovered independently by elementary particle theorists. Their objective has been to practice on models showing confinement and asymptotic freedom in the hope that techniques may be of value for the more physical four dimensional theories. By now it has the appearance of a mature field. But it is too much to expect that such a tidy picture of low-dimensional physics will persist. Already a number of models, that cannot be solved immediately by these methods, are being investigated--that is a symptom of a healthy field.

REFERENCES

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[1] Aubry, S., in Solitons and Condensed Matter Physics, Edited by Bishop A. R. and Schneider, T. (Springer-Verlag, Berlin, Heidelberg, New York, 1978).
[2] Little, W. A., Phys. Rev. 134A (1964) 1416-1424.
[3] See for example articles in Chemistry and Physics of One Dimensional Metals, Edited by Keller, H. J. (Plenum, New York, 1977); Molecular Metals, Edited by Hatfield, W. E. (Plenum, New York, 1979).
[4] Cross, M. C. and Fisher, D. S., Phys. Rev. B19 (1979) 402.
[5] Emery, V. J. and Axe, J. D., Phys. Rev. Lett. 40 (1978) 1507.
[6] For a review see Heeger, A. J. and MacDiarmid, A. G. in Molecular Metals, reference 3, p. 419.
[7] Proceedings of the Kyoto Summer Institute 1979-Physics of Low-Dimensional Systems, edited by Nagaoka, Y. and Hikami, S. (Publication Office, Progress of Theoretical Physics, 1979).
[8] Ordering in Two Dimensions, Edited by Sinha, S. K. (North Holland, New York, Amsterdam, Oxford, 1980).
[9] Potts, R. P., Proc. Camb. Phil. Soc. 48 (1952) 106.
[10] Wegner, F. J., J. Phys. C5 (1972) L131.
[11] See e.g. Emery, V. J. and Swendsen, R. H., Phys. Rev. Lett. 39 (1977) 1414.
[12] For a review see M. P. M. den Nijs, J. Phys. A12 (1979) 1857.
[13] Temperley, H. N. V. and Lieb, E. H., Proc. Roy. Soc. London Ser. A322 (1971) 251.
[14] Jose, J. V., Kadanoff, L. P., Kirkpatrick, S. and Nelson, D. R., Phys. Rev. B16 (1977) 1217.
[15] van Beijeren, H., Phys. Rev. Lett. 38 (1977) 993.
[16] Chui, S. T. and Weeks, J. D., Phys. Rev. B14 (1976) 4978.
[17] This is a very common method of solving problems in two-dimensional statistical mechanics, specific examples are given in references 13 and 23.
[18] Formally this is correct in the limit of strong coupling in one direction and weak coupling in the other. It is often used as an approximate procedure to find a Hamiltonian with the same critical properties as the classical model. A more detailed discussion is given in reference 19.

[19] Black, J. L. and Emery, V. J., Phys. Rev. B23 (1981) 429 and article to be published.
[20] For a review see Fowler, M. in Physics in One Dimension, Edited by J. Bernasconi and Schneider, T., Springer Series in Solid-State Sciences (Springer, Berlin, Heidelberg, New York, 1980).
[21] Dashen, R. F., Hasslacher, B. H. and Neveu, A., Phys. Rev. D11 (1975) 3424.
[22] Johnson, J. D., Krinsky, S. and McCoy, B. M., Phys. Rev. A8 (1972) 2526.
[23] Schultz, T. D., Mattis, D. C. and Lieb, E. H., Rev. Mod. Phys. 36 (1964) 856.
[24] Emery, V. J. in Highly Conducting One-Dimensional Solids, p. 247, Edited by de Vreese, J. T., Evvard, R. P. and van Doren, V. E. (Plenum, New York 1979).
[25] Emery, V. J. in Proceedings of the Kyoto Summer Institute 1979, p. 1 (reference 7).
[26] Luther, A., Phys. Rev. B15 (1977) 403.
[27] Moving along the line of critical points may correspond to changing the temperature, or parameters of the model such as vertex weights or the number (q) of states of the Potts model. Thus the various models may have different exponents because they are related to different points on the critical line.
[28] See for example Introduction to the Renormalization Group and Critical Phenomena, Pfeuty, P. and Toulouse, G. (Wiley, New York 1977).