Excitations in Disordered Systems

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PREFACE

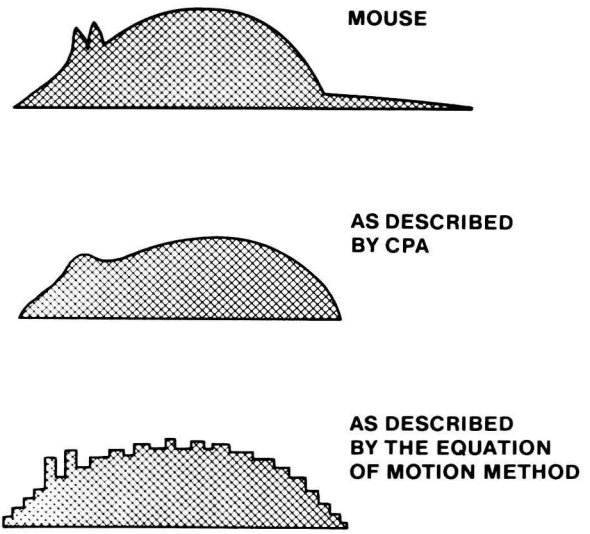
This book has its origin in the NATO Advanced Study Institute held from August 23 - September 4, 1981 at Kellogg Center on the campus of Michigan State University.

The purpose of the school was to survey the current state of understanding of excitations in disordered systems and to provide an update of an earlier influential review article by R. J. Elliott, J. A. Krumhansl and P. L. Leath [Rev. Mod. Phys. 46, 465 (1974)]. The first week of the school concentrated on introductory lectures and the second week on more advanced seminars. They are all published in these proceedings.

The organizers decided to limit the scope of the material to make it manageable and as a result many areas of current interest that are peripheral to the subject were excluded. The common theme throughout is a description of those properties that can be directly understood in terms of elementary excitations. This of course necessitates a good prior knowledge of the structure. Largely excluded from discussion were phase transitions, percolation theory, etc. Other areas such as spin glasses were kept limited in scope.

The book is divided into eight sections. Apart from the Introduction and Summary, each section contains introductory lecture(s) first and more advanced seminars later.

The coherent potential approximation (C.P.A.) has played an important role in our understanding of this area. It is interesting to note that it was first written down by J. C. Maxwell in 1873 for random macroscopic systems (see page 651). Since 1974, numerical methods have had a great influence and there was much discussion as to whether these should be regarded as 'theories' or 'experiments'. Perhaps more illuminating is to regard them as useful half-way houses but that in cases where the physics is clear (e.g. excitations in random magnetic insulators) it is probably not necessary to construct approximate analytic theories. In other cases [e.g. localization] it is desirable and necessary.



Sketch showing the current status of various theories. While the agreement between the objects is not perfect, it should be noted that a mouse, a hippopotamus, and a hedgehog are all mammals. [Kindly provided by D. Weaire.]

The school gave workers in different areas the chance to compare techniques (both experimental and theoretical) and to gauge the relative sophistication of their area.

As well as providing an update on areas that have been studied for some time, two newer areas were covered in some detail. Spin glasses provide a formidable challenge because of the complicated nature of the ground state and localization where numerical methods have been useful in providing leads at this time when no overall understanding has been yet achieved.

In reading through these proceedings, I believe that the only major area that has not been adequately covered is amorphous semiconductors. Much progress was made in understanding these materials in the early seventies and most attention is now being given to the use of hydrogenated amorphous silicon (see page 623) and the fabrication of devices (particularly solar cells).

A summer school like this provides an invaluable opportunity for workers in different areas and at different levels to get together in a relaxed atmosphere. Memories range from the Italian wedding that delayed dinner, to the imaginative refereeing of the

soccer game, to the donuts that weren't donuts, to the modern dance with three witches and a maiden.

I should like to thank our sponsors for their generosity and the organizing committee for their time and expertise. The following faculty and students at Michigan State University also generously contributed their time: R. Barrio, J. Cowen, E. Garboczi, M. Haerle, S. K. Hark, M. J. Harrison, V. Heinen, J. Huffman, C. Lambert, S. D. Mahanti, D. Sahu, J. Shell, M. Thomsen, P. Vora, A. Walker and J. Zwart. I should also like to thank Ms. Delores Sullivan, who was involved in helping to organize the institute, and E. Garboczi, C. Lambert, A. B. Walker and P. Vora for help with these proceedings.

M. F. Thorpe
East Lansing, Michigan
October 1981

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PART I. INTRODUCTION

EXCITATIONS IN DISORDERED SYSTEMS

INTRODUCTORY LECTURES

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1. GENERAL

It is normal to have some disorder in the composition and/or the structure of condensed matter. But until comparatively recently, the theoretical emphasis in solid state physics was on perfect periodic crystals. This was partly because many physical processes can be adequately identified and described in these ideal conditions, but also because the high degree of translational symmetry gives an enormous simplification in the theory so that the elementary excitations are characterised by a wave vector $\underline{k}$ within the Brillouin zone. Even a small amount of disorder destroys the symmetry, and hence these labels for the normal modes, and makes the techniques useless.

In these lectures we discuss the elementary excitations of rigid stable or metastable disordered atomic structures, i.e. mixed crystals or alloys, amorphous solids and glasses. Although the disorder of the latter is similar to that found in the liquid state, the existence of diffusive motions makes the theory of liquids even more difficult. We shall first draw out the mathematical similarities of a range of different excitations although subsequently the main discussion will be of typical fermion and boson systems. Phonons (Taylor) and Spin Waves (Cowley) will be discussed in more detail by other lecturers.

Several reviews [1,2,3] and Ziman's book [4] give an overview of the development of this subject. The discussion here follows that of Elliott, Krumhansl and Leath [1].

2. STRUCTURE

One of the basic difficulties in obtaining a theory of excitations in disordered systems derives from the need to have a suitably complete description of the atomic distribution in the system. In fact such a description is impossible in structurally disordered cases in that it requires knowledge of the ν-point atomic correlation functions for all sizes ν, which is only available for the perfectly periodic case. Experimental information is confined to the pair correlation function

$$g_2(\underline{R}) = \frac{1}{N} \sum_{R_1} n_2(\underline{R}_1, \underline{R}_2)\ \delta\ (\underline{R}_1 - \underline{R}_2 - \underline{R}). \tag{2.1}$$

$g_2(R)$ is the probability of finding an atom at site $\underline{R}$ if there is an atom at the origin. $n_\nu(\underline{R}_1, \underline{R}_2\ ..\ \underline{R}_\nu)$ is the probability of finding ν atoms at $R_1 \ldots R_\nu$ etc. $g_2(R)$ can be measured directly by neutron and X-ray diffraction. Little is known directly about the higher order correlation functions except from model building. For analytic purposes it is necessary to adopt some sweeping approximation such as Kirkwoods Superposition which takes

$$g_3(\underline{R}, \underline{R}') \sim g_2(\underline{R})\ g_2(\underline{R}')\ g_2\ (\underline{R} - \underline{R}') \tag{2.2}$$

(where g_3 is the probability of finding atoms at $\underline{R}$ and $\underline{R}'$ when an atom is present at the origin), and builds up g_ν accordingly (5).

Amorphous and glassy materials usually have strongly directional co-valent bonding where the number and distance of the nearest neighbors is fixed though the bond angles may vary slightly. Thus in pure amorphous Si all atoms may be expected to have four neighbours in an approximately tetrahedral arrangement. However the connectivity of the whole lattice will be variable. For example in the diamond lattice there are six membered rings so that one can return to the origin by well defined self avoiding walks of 6-steps. In amorphous material one may expect 5 and 7 membered rings to occur. It can be shown that many of the salient properties of the excitation spectrum depend mainly on the near neighbour tetrahedral co-ordination and are less affected by the disorder at longer range (cf Weaire lectures). Thus it is sometimes convenient to make very simple approximations about the more distant correlations, as for example, by using the Bethe lattice (Cayley Tree) which has no closed loops (see Thorpe lectures).

Moreover this dependence on local order means that it can be valuable to use methods to describe the excitation spectra which emphasise the local properties such as the Recursion Method (Haydock) and the Continued Fraction Method (Cyrot-Lackmann).