PROPOSAL FOR THE CREATION OF A BAND THEORY PROJECT

" This is a fundamental area of solid-state physics (meaning the problem of band structure) where computers will have a continuing importance. Although theoretical work on electron structure of solids is very strong in the U.K., this is not backed up by a corresponding computational effort" (Computational Chemistry and Physics, Science Research Council. A joint report based on discussions of the Computational Chemistry and Physics Panel (July 1974) 3.3.3 Band Structure Calculations p. 36.

In what follows we shall argue that the establishment and continuous support of such a computation effort is essential if the strong international position of solid-state research in the U.K. is to be maintained.

I. Background.

Band structure calculations have played a major role in the development of our understanding of the condensed state over the past fifteen years. Here we are not referring merely to the very detailed account that can now be given of a vast amount of Fermi-surface data; casting the net much wider, we are suggesting that all our models representing electrons in liquids and solids, such as the tight binding model, the Anderson model for an impurity, the s-d model, the Hubbard model, etc. are to a large extent based on our experience with band structure calculations.

To appreciate the burden of this remark, one only has to compare the sophistication of the discussion of the properties of such relatively complicated compounds as the nitrides and carbides of transition metals (for which the band structure is fairly well known), with the level of comprehension possible at the moment in the case of the A-15 compounds

which are just as important, but where until recently we did not even know the Fermi energy to better than a factor of two. Moreover, as new materials, (e.g. the layered compounds), become subject to intense study, and as the techniques of band theory are extended to deal with such systems as random alloys or such properties as dielectric functions and total energies, band structure calculations will continue to be the ground, admitedly not always solid, on which our theoretical structures have to rest. Significantly, the complex data provided by such modern experimental tools as angle resolved photo-emission spectroscopy becomes useful and detailed information only if the experiment is performed in conjunction with band structure calculations.

Viewed in this light it must be regretted that after a strong initial interest (Altman, Dalton, Goodings, Heine, Hubbard, Zimon) first principles band theory efforts in the U.K. are now not very impressive. The initiative has passed almost exclusively to groups working in the United States: Slater in Florida and M.I.T., Mattheiss at Bell Labs., Koelling Mueller at Argonne., Williams and Janak at I.B.M., Faulkner at Oak Ridge, Switendick at Sandia, Papaconstantopoulos at the Naval Research Laboratory Herman at I.B.M., San Jose, Collins, Wright, Patterson, Kuntz at Urbana, to recall but the largest and most active groups. This situation is unfortunate because over the past decade or so these groups have built up an arsenal of large, efficient programs and a great deal of computational expertise which is not readily available to British workers in need of band theory information. Furthermore, and this must be stressed, such large scale numerical efforts also generate a "quantitative feel" for the 'canonical variables' in the problem, and this is also difficult to come by in the U.K.

What concerns us here is the impact on the American solid state physicist community of having these large and active band theory groups scattered about the country. Though there is no survey to this effect even a superficial look, and a not necessarily admiring one, would result in the

following two observations:

(a) there are many more experimentalists and non-band-theorist theorists who do their own band structure calculations in the U.S. than in the U.K.

(b) experimental papers more frequently have as one of their authors a band theorist who has done the calculation which goes with the experiment being reported.

How this comes about is easy to see. Most American solid state physicists have within easy distance (more in the sense of personal contacts than in miles) a band theory group where they can obtain and learn to run the more or less routine programs for which the need arises in their research. With expert advice and guidance this is not such a great trouble. If more than just routine work is required there is always easy to find a band theorist who is willing to collaborate. It is all informal and as with most such arrangements it works very well. It is our contention that if such help, guidance and opportunity was available to British solid state physicists there would be many happy takers. It is not possible or indeed defensible to set a graduate student the task of producing band theory programs to meet a local and urgent need. Without detailed expert advice such duplication of effort would be a serious waste of scientific manpower and of little educational value. For a novice, even if he is an experienced scientist and programmer such a job can easily take a year and the result is likely to be only second best. Furthermore, the trouble with occasional uses when there are no practicing band theorists around to maintain continuity is that even when someone takes the trouble of writing a useful program he is usually not available to guide the next would be user.

In short, band theory programs are tools, rather like off-the-shelf experimental equipment, and should be used to do physics with. Their lack of availability to British solid state physicists is now a serious handicap. It is to remedy this unfortunate situation that we propose the establishment and continuous funding of a Band Theory Project. Interestingly enough, a

number of European countries have come to the same conclusion in the last three or four years. In order to aid the solid state physics community a band theory centre was set up in Sweden about three years ago. It is run by Dr. Gunner Arbman with the help of several research assistants at the National Defence Research Institute in Stockholm. The role played by this project is very similar to that which we are proposing. Feeling the need for band theory "know-how" particularly among experimentalists has resulted in a new chair being created at the University of Nijmegen in Holland and the appointment of a distinguished American band theorist from Argonne National Laboratories. Very much the same role is played by C. Sommers (again an American import) at Orsay in France and by O. K. Andersen in Copenhager Denmark.

II The way the "Band Theory Project" would work.

The support which the BTP could offer to the solid state physics community can usefully be discussed under four main headings:

(a) Routine service work.

Here we have in mind work for groups having clearly defined short term aims which the BTP could satisfy without substantial program development, e.g. generation of atomic and crystal potentials, calculation of energy bands and Fermi surface cross-sections. This kind of work requires routine 'turn around' of existing programs. Whilst we use the word routine it is only routine for the experienced band theorist and would have taken substantial and in some cases massive effort for the initiator of the request to obtain for himself. Of course coupled with the provision of the results goes advice of standing of the work in the light of the most recent developments in the field.

(b) Medium term interaction.

Here we consider the situation where some particular group would want to undertake some substantial calculations, more than could be reasonably undertaken on a service basis. Here the BTP could fulfil the dual role of providing the basic soft-ware and of providing a centre to which the research workers involved could come, for a short period, to learn how to operate the programs and to obtain advice as to how to modify the codes to suit their particular purpose.

(c) Collaborative Effort

The BTP would be able to establish full collaborative research projects with both theorists and experimentalists, band theory expertise being provided by the BTP. Such collaboration would not simply involve performing routine calculations, rather it would involve development of the basic theory as well as application of the theory to systems of interest.

In this type of collaborative effort we have the possibility of a creative interplay between theory and experiment which could only benefit both sides.

(d) Advisory capacity.

Although the BTP would possess many of the tools of band theory it could never hope, from internal sources, to fulfil every request for computer soft-ware or specialist knowledge. However, the project would be an ideal intermediary between workers abroad, or existing groups in this country, having the expertise required and the 'client'.

Of particular value in this area would be the ability of the BTP to provide a focal point for attracting visiting band theorists from other countries, thus providing a continuing link between British solid state physics and the most modern band theory techniques. If programs could be obtained the BTP would then assist in the unravelling of what are very often rather idiosyncratic codes. The value of having even an experienced band theorist run complicated codes initially under the supervision of the author of them cannot be over emphasised.

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