THE MANY-BODY PROBLEM

Mallorca International School of Physics
August 1969

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PREFACE

The Mallorca International School of Physics was initiated with the aim of fostering new fields of research in physics in the Spanish Universities as well as consolidating those fields in which research is already being pursued. In addition, a School of this character would benefit many students from other countries.

Students of many countries had the opportunity of listening to nearly 60 especially prepared lectures, by physicists, specialists in their field, as well as making personal contact with them (and amongst themselves) to discuss scientific problems of common interest. As a result, it is reasonable to expect that a regularly constituted school, complementary to others already established in Europe, would benefit the staff and students of the Spanish Universities within a period of two or three years.

The subject of The Many-Body Problem was most appropriate for the first school since it is a topic of immediate interest in many branches of Physics - Statistical Mechanics, Nuclear Physics, Solid State Physics and Plasma Physics. The School was fortunate in obtaining an eminent collection of lecturers and I am most grateful that they could spare some of their valuable time to give the new School such a good start. All the lectures appear in the Proceedings with the exception of those by Professor L. Van Hove and Professor P.C. Martin, whose lectures have previously been published. Consequently, the School and these Proceedings will be of benefit to many.

The topicality and attractiveness of the programme was reflected in the large number of applicants to attend the School and some were no doubt additionally influenced by the siting of the School - on a beautiful island, with an international airport, at a world famous holiday resort renowned for sporting and relaxation facilities.

As I have said, it is essential that the School should be a regular one if it is to produce lasting benefit to Spanish scientists and I hope that the Spanish authorities will continue to look on this endeavour in a sympathetic way.

Finally, I have much pleasure in giving my sincerest thanks to many people who helped to transform the School from an idea to a reality:

Professor J.L. Villar-Palasí, Minister of Education of Spain for sponsoring the School.

Dr. R. Diez-Hochleitner, Secretary General of the Ministry of Education for receiving the project of the School with such enthusiasm.

Professor F. Rodriguez, Director General of Universities in Spain and Dr. A. de Juan-Abad for providing the necessary finance.

Professor G. Tomás , Rector of the Estudio General Luliano, where the lectures were held.

The Majorcan Authorities, who contributed to making the School a success.

Professor Sir Rudolph Peierls, F.R.S. (University of Oxford) for continuous moral support in the organization of the School.

Professor N. Kemmer, F.R.S. (University of Edinburgh), who provided so much useful information on the running of a School of this nature.

Dr. A. Cruz (University of Zaragoza) and Dr. T.W. Preist (University of Exeter) co-editors of the Proceedings.

And finally, Mrs. R.W. Chester (University of Edinburgh) and Miss H.H. Ostermann (University of Barcelona) for their heroic efforts in the typing of the manuscript and the organization of the School.

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EDITORS' NOTE

The lecture notes were prepared by the lecturers themselves before or during the School. The final manuscript was typed during and after the School had finished. As a result most of the lecturers were unable to see it in its final form and consequently the responsibility for any errors and misprints lies with the editors.

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GREEN FUNCTIONS APPLIED TO PHONON PROBLEMS

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I. INTRODUCTION TO DYNAMICS AND TO GREEN FUNCTIONS

1. CRYSTAL AND LIQUID HAMILTONIANS

1.1 Crystal Hamiltonian in Adiabatic Approximation[1,2,3]

We introduce the following notation: N is the number of unit cells in the crystal volume V as defined by periodic boundary conditions, and $\vec{R}_I$ $(I = 1,\dots N)$ are the cell positions. Each cell contains B basis ions $(B = 1$ for a Bravais lattice$)$ with mass M_b and equilibrium position $\vec{R}^o_{Ib}$ $(b = 1,\dots B)$; we fix $\vec{R}^o_{I1} = \vec{R}_I$. The instantaneous positions of the ions are given by $R = \left\{\vec{R}_{Ib} = \vec{R}^o_{Ib} + \vec{u}_{Ib}\right\}$ where $\vec{u}_{Ib}$ are their displacements. Z is the number of valence electrons per cell at temperature $T = 0$ $(Z = 0$ for an insulator$)$ and $r = \left\{r_e\right\}$ $(e = 1,\dots, ZN)$ are the positions of the valence electrons (mass m).

Since m/M_b is always very small $(< 10^{-3})$ the electrons move so fast as to screen the long range Coulomb interaction of the ions. Then the Hamiltonian may be written

$$H = H_{ion} + H_{el} \tag{1.1.1}$$

$$H_{ion} = \sum_{I,b} \frac{\vec{P}_{Ib}^{\,2}}{2M_b} + U(R) \tag{1.1.2}$$

$$H_{el}(R) = \sum_e \left(\frac{\vec{p}_e^{\,2}}{2m} + W(\vec{r}_e, R)\right) + H_{coul} \tag{1.1.3}$$

where H_{coul} is the Coulomb interaction between electrons. In the <u>adiabatic</u> or <u>Born-Oppenheimer approximation</u> the electron dynamics is solved for fixed instantaneous ion positions

$$H_{el}(R)|\ell,R\rangle = E_\ell(R)|\ell,R\rangle \tag{1.1.4}$$

$$\langle \ell',R|\ell,R\rangle = \delta_{\ell\ell'} \tag{1.1.4$'$}$$

and the effect of the ionic kinetic energy on these states is neglected,

$$\langle \ell',R|H|\ell,R\rangle \cong (H_{ion} + E(R))\,\delta_{\ell\ell'} \tag{1.1.5}$$

If the displacements $\vec{u}_{Ib}$ are small compared to the interatomic distances, (1.1.4) may first be solved to zeroth order in the $\vec{u}_{Ib}$ by a Hartree-Fock procedure

$$H_{el}(R^o) = H_{HF} + H_{el-el} - \tfrac{1}{2}\sum_e V_{HF}(\vec{r}_e) \tag{1.1.6}$$

where $V_{HF}(\vec{r}_e)$ is the self-consistent field determined such that the residual electron-electron interaction

$$H_{el-el} = H_{coul} - \tfrac{1}{2}\sum_e V_{HF}(r_e) \tag{1.1.7}$$

does not contribute to the energy of the Hartree-Fock ground state $|\phi_o\rangle$, $\langle\phi_o|H_{el-el}|\phi_o\rangle = 0$.

$$H_{HF} = \sum_e \left(\frac{\vec{p}_e^{\,2}}{2m} + V(\vec{r}_e)\right) \tag{1.1.8}$$

where

$$V(\vec{r}) = W(\vec{r},R) + V_{HF}(\vec{r}) \tag{1.1.9}$$

is the periodic potential, defines free quasi-particles