Correlation Functions and Quasiparticle Interactions in Condensed Matter

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PREFACE

This volume contains the proceedings of a NATO Advanced Study Institute devoted to the study of dynamical correlation functions of the form

$$C_{AB;AB}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} \langle A(o)B(o)A(t)B(t) \rangle dt \qquad (1)$$

where A and B are physical operations in the Heisenberg representation and

$$\langle \ldots \rangle = \frac{Tr(e^{-\beta \mathcal{H}} \ldots)}{Tre^{-\beta \mathcal{H}}}$$

is an equilibrium average. In equation (1) it is useful to regard the product AB as the product of two operators in cases in which A and B refer to different spatial points in a condensed matter system and/or in which A and B behave dynamically in a quasiharmonic way. In the second case, one has a two quasiparticle correlation function and $C_{AB;AB}(\omega)$ gives information about quasiparticle interactions.

Condensed matter physics has increasingly turned its attention to correlation functions of this type during the last 15 years, partly because the two point and/or one-particle correlation functions have by now been very thoroughly studied in many cases. The study of four point and/or two quasiparticle correlations has proceeded somewhat independently in several diverse fields of condensed matter physics and it was one purpose of the institute to bring experts from these different fields together to describe the current state of their art to each other and to advanced students.

The fields represented included solid state physics of phonons and magnons and superconductivity, dynamical critical phenomena and the physics of classical and superfluid liquids. In this volume, the first section contains four lectures on basic theoretical rela-

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tionships and techniques which underlie much of the interpretation of of the physics of the systems discussed in the following sections. These lectures describe basic theory of response functions (R. Stinchcombe), many-body perturbation theory (J.W. Halley), theory of dynamical critical phenomena (G. Mazenko) and the foundations of hydrodynamics (I. Oppenheim). In the next three sections of this volume, studies of correlation functions in magnetic systems, liquids and phonons in solids are described. The identity of the operators A and B in these various fields is indicated in Table 1. Lecturers on these topics were H. Bilz (phonons), R. Cowley (liquids, magnons and phonons), P. Fleury (liquids and magnons), W. Gelbart (liquids), A. Rahman (liquids), I. Silvera (quantum solids) and M. Thorpe (magnons).

Twelve people contributed brief manuscripts on special aspects of the subject on which they gave seminars at the institute. These were M.G. Cottam, U. Balucani and V. Tognetti, and P.D. Loly (magnons), A. Ben-Reuven, D. Frenkel, H. Metiu and R. Kapral (classical liquids), C. Murray, R. Hastings and F. Pinski (superfluid ^{4}He), A. Goldman (superconductivity) and W. Buyers (phonons). Seminars were also given at the institute on superionic conductors (S. Ushioda), phonon bond states (J. Ruvalds) and long time behavior of spin correlation function (D. Huber).

In reviewing the contents of this volume certain impressions emerge. The problem of analyzing experiments which give information on correlation functions of the sort considered here, falls into two parts: 1) The computation of the coupling between the probe (usually electromagnetic radiation or neutrons) and the many-body system and 2) the computation of the correlation function itself.

TABLE 1. Identity of the operators A,B of equation (1) in various systems

STATE	A,B	QUASIPARTICLE
Solid (non-magnetic)	$\underset{\sim}{\rho}^{k}, \underset{\sim}{\rho}^{-k}$	phonons
Solid (magnetic)	$S^{\mu}_{k}, S^{\nu}_{-k}$	spin waves (magnons)
Critical Regions	both above	none
Liquids	$\underset{\sim}{\rho}^{k}, \underset{\sim}{\rho}^{-k}$	phonons and rotons (^{4}He) None (classical)

In magnetic systems for T below the ordering temperature, both aspects of the problem are now under reasonably good control except in the critical region where the techniques described by G. Mazenko have not yet been seriously applied to the sort of correlation functions discussed at the institute. Above the ordering temperature little has been done; the work described by Balucani and Tognetti in this volume is a start. (Work by P. Fedders should also be mentioned in this connection.)

In liquid physics, W. Gelbart describes the problem of computing second order coupling to light in this volume. Large uncertainties remain in this area. It is possible that x-ray scattering experiments could contribute to a resolution of this problem. The problem of the computation of the higher order correlation function in classical liquids is probably amenable to solution by molecular dynamics. Preliminary work is described by A. Rahmann in this volume. (The HNC techniques described by F. Pinski in this volume are useful for integrated scattering but not for the dynamics.) The talk by R. Hastings shows that attempts to calculate dynamical four point response functions in liquid ^{4}He remain at the phenomenological level.

In phonon systems, the reviews by R. Cowley and H. Bilz indicate good qualitative understanding of most higher order phonon spectra and couplings though quantitative microscopic (as opposed to phenomenological) models are not yet available. In quantum solids, as described by Silvera, the basic dispersion relations have not yet been obtained from neutron scattering and this remains a major obstacle to a quantitative understanding of the higher order optical spectra. It remains unclear whether bound states of phonons have been seen in solids. People interested in this question might wish to be more systematic about seeking optimal materials in which to see this phenomenon unambiguously.

Finally, in general response theory it appears that a large area of theoretical development in the area of non-linear optics in condensed matter has only begun to be discussed.

Many people contributed to the success of this institute. I will mention first Professor Charles Campbell who, as local committee chairman, was indispensable and who also contributed in a very important way scientifically. The organizing committee provided indispensable assistance over a period of more than a year. The committee members were Heinz Bilz, Charles Enz, Paul Fleury, William Gelbart, Satoru Sugano, Michael Thorpe. The following local companies contributed financially: Deluxe Check Printers Foundation, Magnetic Controls Company and Northern States Power Company. We also received some aid from the University of Minnesota Graduate School. Indispensable administrative assistance from the office of Associate Dean of the University of

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J. Woods Halley
Minneapolis, Minnesota 1978

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Part I
General Theory

KUBO AND ZUBAREV FORMULATIONS OF RESPONSE THEORY

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ABSTRACT

The theory of the linear response of systems to external adiabatic and isothermal perturbations is reviewed. The relationship of the response coefficient to correlation functions and to Green functions is developed following the work of Kubo and Zubarev. The Green function method is illustrated with examples, and brief treatments are given of sum rules and of the fluctuation-dissipation theorem. It is shown how the framework may be used to discuss quasiparticle and collective modes, equilibrium thermal properties, and cross sections for neutron and electromagnetic scattering.

1. INTRODUCTION

The underlying theme of these lectures is that most properties of systems are closely related to the response of the system to appropriate external 'fields'.

This statement applies to properties ranging from bulk thermal, mechanical and magnetic properties (such as specific heat, compressibility and susceptibility) to those properties, such as phonon and spin wave energies and lifetimes which are characteristic of individual modes of the system.

The relationship is rather obvious for the bulk properties, which are in most cases observed by measuring the effect on the system of temperature changes, or the response to mechanical forces or electromagnetic fields.

It is less obvious for the single mode properties, such as excitation spectra which are usually obtained from the cross section for inelastic scattering of neutrons, electrons or photons, in which the change of state of the scattered particle is associated with a definite energy transfer ω and momentum transfer q to the system. In that case a specific normal mode at frequency ω and wave vector q is probed, so long as the normal mode couples to the scattered particle, and so long as q is a good quantum number for the modes, as is the case for e.g. a perfect crystal*. Whether or not a single mode, or many, are involved, it will be shown that such experiments are closely related to the (adiabatic) response of the system to wave-vector and frequency-dependent external fields, i.e. to "generalised susceptibilities".

Another point to be stressed is the relationship of such "susceptibilities" (response functions) to correlation functions.

The usual bulk isothermal magnetic susceptibility is the ratio of the magnetisation $\partial F/\partial h$ to the applied magnetic field h and is therefore a second derivative of the free energy F with respect to field. Similarly the isothermal compressibility is a second derivative with respect to pressure. As is well known and will be illustrated later such second derivatives are identical to static correlation functions between "macroscopic"operators (the total magnetization operator in the case of magnetic susceptibility.

The bulk adiabatic susceptibility or compressibility is the ratio of the response to the adiabatically applied field or pressure. We shall show, following the original development by Kubo [1], that this type of response coefficient can again be calculated in terms of correlation functions between the same "macroscopic" operators; but in this case a time-dependent correlation function is required. This type of description also applies to transport coefficients such as the electrical conductivity, and generalises immediately to frequency-dependent processes.

---

*

In the case of imperfect crystals, the momentum transfer to the system q will be shared between all the normal modes at frequency ω. A sum over normal modes at a particular energy is again involved in, for example, optical absorption, in which only the energy dependence is measured. In other cases, such as X-ray scattering, the wave vector change is identified but all contributing normal modes, whatever their energies, are summed over, yielding information on the structure but not on the dynamics.

For the generalised susceptibilities involving wave vector as well as frequency dependence, such as those related to scattering by particular normal modes, or to the response to non-uniform time-dependent fields, the related time-dependent correlation function is between operators which carry particular momentum labels.

Sometimes it is convenient to work directly in terms of the generalised susceptibility or the related correlation function. However a compact formalism exists for the calculation of static or time-dependent correlation functions by means of Green function equation of motion methods as described by Zubarev [2] and others [3]. The Green functions depend on two time labels and, like the correlation functions they are designed to lead to, they normally involve also thermal aspects since averaging over some (e.g. canonical) ensemble is involved. Even where the required correlation functions relate to macroscopic properties of the system the Green function method does not require complete normal mode solutions for the system.

We proceed at once (Section 2) to a statement of Kubo's theory of adiabatic linear response. This is followed by a brief section (§3) on isothermal response. In these two sections the relationship between response functions and correlation functions appears. The two-time Green function is then introduced and related to the correlation function (Section 4). In Section 5, simple examples are given to illustrate the main points previously discussed. After a short section (§6) on other types of Green function, the direct relationship between Green functions and normal mode properties is then exhibited (§7). Section 8 contains formal properties, such as sum rules, while Section 9 derives and discusses the importance of the fluctuation-dissipation theorem. The following section (§10) treats the various scattering processes which allow the normal modes to be probed, and the relationship of cross-sections to the correlation functions. The concluding section (§11)gives some generalisations of the previous discussions, and refers to situations where a breakdown of the linear response approach could occur.

2. KUBO FORMULA FOR LINEAR RESPONSE [1,4]

(i) Response function

The linear response of a system to an adiabatically applied external field F(t) may be easily derived as follows when the field can be introduced by means of an additional term in the Hamiltonian, of the form

$$H_1 = - AF(t) \qquad (2.1)$$

Here A is the operator to which the field linearly couples (e.g. a dipole operator if F is a uniform electric field, or a magnetic moment if F is a magnetic field).

It is supposed that the response to the field is observed by measuring the change ΔB it produces in the mean value of a particular operator B (e.g. a current operator). Such mean values can be obtained from the density matrix $\rho(F)$ for the system in the applied field

$$\rho(F) = \rho + \delta + O(F^2). \tag{2.2}$$

ρ and δ are here the zeroth and first order terms respectively in the expansion of $\rho(F)$ in powers of F. The linear response is then

$$\Delta B \equiv Tr\ \delta B \tag{2.3}$$

If H is the Hamiltonian of the system in zero field, $\rho(F)$ satisfies (taking $\hbar = 1$)

$$\dot{\rho}(F) = -i\,[(H+H_1), \rho(F)] \tag{2.4}$$

from which the terms linear in the applied field are

$$\dot{\delta} = -i\,[H, \delta] + i\,[A, \rho]\,F(t). \tag{2.5}$$

This has the formal solution

$$\delta(t) = i\int_{-\infty}^{t} dt'\, e^{iH(t'-t)}\,[A,\rho]\,F(t')\,e^{-iH(t'-t)} \tag{2.6}$$

where use has been made of $\delta(-\infty) = 0$, since the field was switched on adiabatically from zero in the distant past. Inserting (2.6) into (2.3) and using cylic invariance within the trace and the usual definition of Heisenberg operators gives the linear response at time t

$$\Delta B \equiv Tr\,\delta B = \int_{-\infty}^{t} \phi_{BA}(t-t')\,F(t')\,dt' \tag{2.7}$$

where ϕ_{BA} is the "response" or "after-effect" function

$$\phi_{BA}(t) = i\,Tr\,[A,\rho]\,B(t) = i\,\langle [B(t), A] \rangle \tag{2.8}$$

where

$$B(t) = e^{iHt}\,B\,e^{-iHt}, \tag{2.9}$$

and

$$\langle \ldots \rangle = Tr\,\{\rho \ldots\} \tag{2.10}$$

is the usual zero field average.

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