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Student Days

Rex Godby, University of York

G staircase 1978-1981

G staircase 1978-1981

Supervisors

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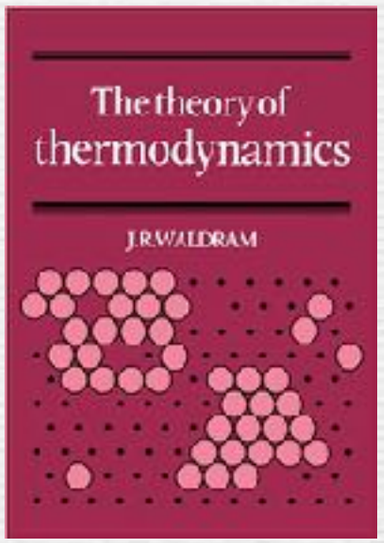
John Waldram (Physics; DoS)



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Roger Haydock (Physics)

Supervisors

Richard Stibbs
(Maths for Nat. Sci.)

John Samson (Quantum Mechanics)

Cavendish Laboratory

PhD 1981-1984: TCM

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John Inkson

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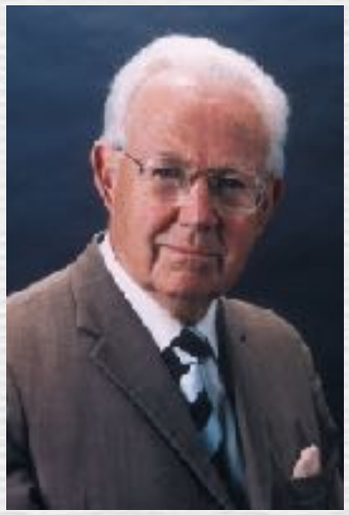
Volker Heine



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Sam Edwards

J. Phys. C: Solid State Phys., **16** (1983) L291–L299. Printed in Great Britain

LETTER TO THE EDITOR

Energy loss rate in silicon inversion layers

M C Payne, R A Davies†, J C Inkson and M Pepper‡
Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 6 January 1983

Abstract. We report the results of measurements on the rate of heat loss from hot electrons in silicon inversion layers at low temperatures. The results are interpreted in terms of the generation of acoustic phonons and it is found that disorder has a significant effect on this mechanism. In the low-disorder, high-temperature limit the energy relaxation time τ_ϵ varies with electron temperature T_e as T_e^{-4}. In the high-disorder, low-temperature limit τ_ϵ varies as T_e^{-2}. The electron temperature is measured by the effect on the weak two-dimensional localisation which allows the experiment to be performed at low temperatures.

J. Phys. C: Solid State Phys., **16** (1983) 4259–4272. Printed in Great Britain

Inelastic electron tunnelling spectroscopy

M C Payne and J C Inkson
Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 4 February 1983

Abstract. Experiments have used inelastic electron tunnelling spectroscopy as a method of measuring the phonon density of states of the tunnelling barrier. The magnitude of the measured d^2I/dV^2 characteristic is proportional to the density of phonon states multiplied by a weighting factor, which depends on the strength of the interaction between the electron and the phonon. Without a knowledge of this weighting factor the experiments can only yield qualitative results. In this paper we present a study of the tunnelling process and derive a weighting factor which allows the phonon density of states to be deduced from the experimental data.

+ Density-Functional Theory!

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R.O. Jones

TCM Seminar 1982

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{2}{3}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

I. INTRODUCTION

IN recent years a great deal of attention has been given to the problem of a homogeneous gas of interacting electrons and its properties have been established with a considerable degree of confidence over a wide

In Secs. III and IV, we describe the necessary modifications to deal with the finite-temperature properties and with the spin paramagnetism of an inhomogeneous electron gas.

Of course, the simple methods which are here proposed in general involve errors. These are of two general

Physica Scripta. Vol. 21, 394–401, 1980

Density Functional Calculations for Atoms, Molecules and Clusters

O. Gunnarsson and R. O. Jones

Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-5170 Jülich, Germany

Received June 12 1979

Abstract

Density functional calculations for atoms, molecules and clusters. O. Gunnarsson and R. O. Jones (Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-5170 Jülich, Germany).
Physica Scripta (Sweden) 21, 394–401, 1980.

The density functional formalism provides a framework for including exchange and correlation effects in the calculation of ground state properties of many-electron systems. The reduction of the problem to the solution of single-particle equations leads to important numerical advantages over other ab initio methods of incorporating correlation effects. The essential features of the scheme are outlined and results obtained for atomic and molecular systems are surveyed. The local spin density (LSD) approximation gives generally good results for systems where the bonding involves *s* and *p* electrons, but results are less satisfactory for *d*-bonded systems. Non-local modifications to the LSD approximation have been tested on atomic systems yielding much im-

$$n(r) = \sum_{i=1}^{N} |\psi_i(r)|^2 \tag{3}$$

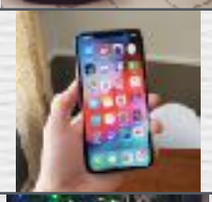
where the xc-potential, $v_{xc}(r)$, is the functional derivative

$$v_{xc}(r) = \frac{\delta E_{xc}[n]}{\delta n(r)} \tag{4}$$

and N is the number of electrons. This approach gives the ground state density $n(r)$ and the total energy $E_v[n]$, as well as properties which can be derived from them. The ϵ_i's are Lagrange parameters and have not been shown to have any direct physical meaning. There is, for example, no analogue to Koopmans' theorem of Hartree–Fock theory.

Equation (2) is a one-body equation, so that the N-particle

+ Computing Power!

Computer	Memory (MB)	Speed (Gflops)	Cost (£, [2020 £])
1978: IBM 370/165 (Phoenix) 	1	0.001	£1M [£4M]
1981: Cray-1 	8	0.2	£5M [£15M]
2020: iPhone 	2000	100	£500
2020: medium cluster (1000 cores) 	2,000,000	50,000	£0.5M

Pembroke Fellow 1984-

MIT 1985-6

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The Rest is History!