Springer Theses Recognizing Outstanding Ph.D. Research

Mark Edward Barber

Uniaxial Stress Technique and Investigations of Correlated Electron Systems



Springer Theses

Recognizing Outstanding Ph.D. Research

Aims and Scope

The series "Springer Theses" brings together a selection of the very best Ph.D. theses from around the world and across the physical sciences. Nominated and endorsed by two recognized specialists, each published volume has been selected for its scientific excellence and the high impact of its contents for the pertinent field of research. For greater accessibility to non-specialists, the published versions include an extended introduction, as well as a foreword by the student's supervisor explaining the special relevance of the work for the field. As a whole, the series will provide a valuable resource both for newcomers to the research fields described, and for other scientists seeking detailed background information on special questions. Finally, it provides an accredited documentation of the valuable contributions made by today's younger generation of scientists.

Theses are accepted into the series by invited nomination only and must fulfill all of the following criteria

- They must be written in good English.
- The topic should fall within the confines of Chemistry, Physics, Earth Sciences, Engineering and related interdisciplinary fields such as Materials, Nanoscience, Chemical Engineering, Complex Systems and Biophysics.
- The work reported in the thesis must represent a significant scientific advance.
- If the thesis includes previously published material, permission to reproduce this must be gained from the respective copyright holder.
- They must have been examined and passed during the 12 months prior to nomination.
- Each thesis should include a foreword by the supervisor outlining the significance of its content.
- The theses should have a clearly defined structure including an introduction accessible to scientists not expert in that particular field.

More information about this series at http://www.springer.com/series/8790

Mark Edward Barber

Uniaxial Stress Technique and Investigations of Correlated Electron Systems

Doctoral Thesis accepted by the University of St Andrews, St Andrews, UK



Author Dr. Mark Edward Barber School of Physics and Astronomy University of St Andrews St Andrews UK Supervisors Prof. A. P. Mackenzie Max Planck Institute for Chemical Physics of Solids Dresden Germany

Dr. C. W. Hicks Max Planck Institute for Chemical Physics of Solids Dresden Germany

 ISSN 2190-5053
 ISSN 2190-5061
 (electronic)

 Springer Theses
 ISBN 978-3-319-93972-8
 ISBN 978-3-319-93973-5
 (eBook)

 https://doi.org/10.1007/978-3-319-93973-5
 ISBN 978-3-319-93973-5
 (eBook)

Library of Congress Control Number: 2018945099

© Springer International Publishing AG, part of Springer Nature 2018

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Printed on acid-free paper

This Springer imprint is published by the registered company Springer International Publishing AG part of Springer Nature

The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Supervisors' Foreword

It was a real pleasure to supervise Mark Barber's Ph.D. research. Mark came to St Andrews in 2012 with excellent qualifications from the University of Cambridge, and his exceptional abilities soon became clear to us. When set a high-level research task, Mark quickly understands on his own what is needed and almost always returns with solutions rather than further questions.

Mark quickly began to make major contributions to the main theme of the group's work at that time, the development of a new technique for the application of uniaxial pressure. In those early stages, calculations were required in order to understand how to achieve the most homogeneous strain fields in the samples. Rather than try to purchase commercial software, Mark wrote a package to perform finite element calculations from scratch. He not only achieved this very quickly but also designed the package so that it was adaptable and easy for him to use on a host of related problems. The calculations strongly influenced the way that the samples were mounted for the 2013 and 2014 experiments, hence making a major contribution to their success.

After this excellent start to his research, he faced what most graduate students would regard as an unwelcome disruption, as we relocated our group from St Andrews to the Max Planck Institute for Chemical Physics of Solids in Dresden, Germany. Given the choice to stay working with existing equipment in St Andrews or come to the new environment, he was clear both that he wanted to move and that he would like to take on a major experimental task. We had the funds to purchase two new cryostats, to be installed in a brand new laboratory in Dresden. Mark asked to be involved in the specification at the prepurchase stage but also to be given the responsibility to commission the cryostats and associated electronics. This is a big job, especially when one includes the demands of designing and writing a full data acquisition package, but such is Mark's ability that we agreed, as long as we could monitor his progress. Needless to say, what he produced exceeded any reasonable expectations. Within less than a year from an empty laboratory, he was simultaneously performing experiments on both cryostats, having written more or less autonomous software that took data, performed initial online analysis of it, and used

the information to "decide" on the next run. If human intervention was needed, it sent him a message telling him what was required.

The semiautonomous software was a nice touch, but nothing that Mark does is purely for show. It enabled him to build up two major data sets in an incredibly short space of time. The first, on the unconventional superconductor Sr_2RuO_4 , he showed both that it is possible to drive it through a topological transition of its Fermi surface with uniaxial pressure, and that its superconducting transition temperature peaks sharply at approximately the same strain. These were world first results, leading to the publication of several papers. In his second piece of original research, he demonstrated the sensitivity to uniaxial pressure of the novel magnetic and possibly nematic order in the related material $Sr_3Ru_2O_7$. Mark also contributed strongly to research on the high-temperature superconductor $YBa_2Cu_3O_{6+x}$ under uniaxial stress, a notable effort as it required detailed collaboration with other groups.

For parts of the Sr_2RuO_4 research, the high purity of the single crystals led to difficulties in measuring their extremely low resistances accurately. Mark and a colleague noted that this was due to a deficiency in standard current sources, and designed and built a new one, described in the thesis, to overcome the problem. This quiet determination, coupled with high ability and creativity, are Mark's defining characteristics as a scientist. Like most really good researchers, he is also unselfish and always willing to help others, both within the group and beyond. We have had a string of visitors, keen to learn the tricks of the new techniques. Mark is always willing to help them, and having seen him at work, they regularly tell us how impressed they are with quality of what he does. Having explained his work many times in person, he realized the importance of the didactic part of his thesis, and took considerable care to write a document that would help others around the world who wish to set up similar experiments.

In summary, Mark has been an outstanding graduate student, with whom it has been a pleasure to work, and this is in our opinion an outstanding thesis.

Dresden, Germany March 2018 A. P. Mackenzie C. W. Hicks

Abstract

In the repertoire of an experimental condensed matter physicist, the ability to tune continuously through features in the electronic structure and to selectively break point-group symmetries are both valuable techniques. The experimental technique at the heart of this dissertation, uniaxial stress, can do both such things.

The thesis will start with a thorough discussion of our new technique, which was continually developed over the course of this work, presenting both its unique capabilities and also some guidance on the best working practices, before moving on to describe results obtained on two different strongly correlated electron materials.

The first, Sr_2RuO_4 , is an unconventional superconductor, whose order parameter has long been speculated to be odd-parity. Of interest to us is the close proximity of one of its three Fermi surfaces to a Van Hove singularity (VHs). Our results strongly suggest that we have been able to traverse the VHs, inducing a topological Lifshitz transition. T_c is enhanced by a factor ~ 2.3 and measurements of H_{c2} open the possibility that optimally strained Sr_2RuO_4 has an even-parity, rather than odd-parity, order parameter. Measurements of the normal state properties show that quasiparticle scattering is increased across all the bands and in all directions, and effects of quantum criticality are observed around the suspected Lifshitz transition.

 $Sr_3Ru_2O_7$ has a metamagnetic quantum critical endpoint, which in highly pure samples is masked by a novel phase. Weak in-plane magnetic fields are well-known to induce strong resistive anisotropy in the novel phase, leading to speculation that a spontaneous, electronically driven lowering of symmetry occurs. Using magnetic susceptibility and resistivity measurements, we can show that in-plane anisotropic strain also reveals the strong susceptibility to electronic anisotropy. However, the phase diagram that these pressure measurements reveal is consistent only with large but finite susceptibility, and not with spontaneous symmetry reduction.

Acknowledgements

The work this thesis represents amounts to almost 4 years of study, spanning two different institutions, all of which would not have been possible had it not been for the great number of colleagues and friends alike who have helped and supported me throughout.

First and foremost I would like to thank Andy Mackenzie, my supervisor, for his guidance and support along the way. His unique perspective on physics has been incredibly enlightening and I have learnt a great deal. I am also particularly grateful that Andy gave me the time to explore these new ideas in my own way.

None of the work in this thesis would have been possible without the ingenuity of Clifford Hicks and to him I would like to express my sincere gratitude. Not only did he instigate the whole the uniaxial stress project but he has also provided invaluable support, physical insight, and supervision throughout my measurements.

During my Ph.D., I have been fortunate enough to spend time at the University of St Andrews and the Max Planck Institute for Chemical Physics of Solids where I have benefited in different ways from a great number of people. There are too many to thank explicitly here, but I would like to mention just a few in particular. The technical staff of the mechanical workshops and Ulrike Ließ who built the devices were pivotal in the success of this technique, and so too were the cryogenics staff. As part of the Condensed Matter Centre for Doctoral Training, I am particularly indebted to the administrative staff, Christine Edwards, Julie Massey, and Wendy Clark, who made everything run so smoothly and were especially accommodating with my move to the MPI.

From the lab, I am thankful to Dan Brodsky and Jan Bruin who first introduced me to the adiabatic demagnetization refrigerator. I did not ultimately use this cryostat for my final measurements, but it is the one on which I got to work on the strain project for the first time, in collaboration with Dan.

During the middle of my Ph.D., I worked on a series of measurements on the cuprates with Nabhanila Nandi and Chufo Borzi. Despite these measurements not making the final cut for inclusion in this thesis, I am particularly grateful for the useful discussions we had together and for making my time in the lab, and Dresden,

especially enjoyable. I would also like to thank Veronika Sunko who helped out at the start of the $Sr_3Ru_2O_7$ measurements.

Finally, I would like to thank my family who have always been supportive of my studies and have helped me to reach where I am today, and also Nabhanila for her continued support and encourgament that helped me complete this thesis.

I would like to acknowledge financial support from the Engineering and Physical Sciences Research Council via the Scottish Condensed Matter Centre for Doctoral Training under grant EP/G03673X/1, and from the Max Planck Society.

Contents

1	Introduction						
	1.1	Electrons in Metals					
	1.2	Landau's Fermi Liquid					
	Refe	References					
2	Uniaxial Stress Technique						
	2.1	Introduction	13				
	2.2	Stress and Strain	14				
	2.3	Finite Element Method	17				
	2.4	Uniaxial Stress and Strain Techniques	20				
		2.4.1 Indirect Determination Using Ehrenfest Relations	20				
		2.4.2 Anvil-Based Pressure Cells	22				
		2.4.3 Sample on Piezo Stack	24				
		2.4.4 Other Techniques.	27				
	2.5	New Uniaxial Stress Cell	27				
		2.5.1 Sample Mounting	31				
		2.5.2 Sample Mounting Models	36				
	2.6	Recommended Working Parameters 4					
	2.7	Conclusions	43				
	Refe	rences	45				
3	The	Physics of Sr ₂ RuO ₄ Approaching a Van Hove Singularity	49				
	3.1	Introduction	49				
	3.2	Background Physics for Sr ₂ RuO ₄	51				
		3.2.1 Fermi Liquid Properties of Sr ₂ RuO ₄	51				
		3.2.2 Superconductivity of Sr_2RuO_4	54				
		3.2.3 Van Hove Singularities and Lifshitz Transitions					
		and Their Connection to Sr ₂ RuO ₄	68				
	3.3	Experimental Methods	74				
	3.4	Results and Discussions	82				

		3.4.1	Superconducting Properties Under Strain	82		
		3.4.2	Normal State Properties Under Strain	90		
	3.5	Conclu	usions	103		
	Refe	rences		104		
4	Oua	ntum (Criticality and Metamagnetism of Strained			
-	Sr ₃ F	Ru_2O_7		111		
	4.1	Introdu	uction	111		
	4.2	Backg	round Physics for Sr ₃ Ru ₂ O ₇	112		
		4.2.1	Itinerant Metamagnetism	115		
		4.2.2	Quantum Criticality	120		
		4.2.3	Novel Ordered Phase	124		
		4.2.4	Latest Developments and Motivation	129		
	4.3	Experi	mental Methods	130		
		4.3.1	Sample Preparation	131		
		4.3.2	Resistivity Measurements	132		
		4.3.3	Magnetic Measurements	137		
		4.3.4	Strain Transmission	139		
		4.3.5	Low Temperature Cryostat	139		
	4.4	Result	s and Discussions	142		
		4.4.1	Magnetoresistance	142		
		4.4.2	Metamagnetism	146		
		4.4.3	Strain Ramps	150		
		4.4.4	Higher Temperatures	151		
		4.4.5	Discussion	155		
	4.5	Conclu	usions	159		
	Refe	rences		160		
5	Conclusions and Outlook					
	References					
4	nond	: А. Г	Details of the Dual End Cumunt Source with Active			
Common-Mode Rejection						
Common-Moue Rejection						
Ар	pend	ix B: S	upplementary Materials for Sr ₂ RuO ₄ Under Strain	173		
Ар	pend	ix C: P	hase Boundaries from the Derivatives of Resistivity			
		iı	n Sr ₃ Ru ₂ O ₇	183		
Ар	Appendix D: AC Susceptibility Coils Simulation					

Chapter 1 Introduction



The interactions between particles in nature can present a bewildering array of exotic states and phenomena, each fascinating in their own right, but also in terms of their potential applications. Condensed matter systems with as many as 10^{22} atoms in a single cubic centimetre are a prime example. Of interest for this thesis are a group of materials in which the interactions between electrons are particularly strong, such that one must consider the behaviour of the electrons as correlated. These interactions can drive the formation of states such as superconductors, strange metals and a variety of different magnetic states, to name just a few.

To understand the behaviour of a complex system one often turns to the individual building blocks. In condensed matter physics these are the atoms making up the solid. When considering metals we are concerned with the positive ions which form the crystal lattice and the conduction electrons that move through it. The positive ions comprise the nuclei of the constituent atoms plus the core electrons. The conduction electrons are the outer most electrons which can lower their kinetic energy by travelling through the lattice. This energy benefit is key to the cohesion of atoms in metals [1].

It is simple to account for the motion of each of the individual building blocks and the Coulomb interactions between them but this fully reductionist approach runs into complications [2]. The equations can describe a vast number of properties in condensed matter but the interaction terms put exact solutions for all but the simplest systems out of reach. Instead we must simplify the situation and look for 'emergent' phenomena. As experimentalists we can try to understand these emergent states by measuring their physical properties, but given the ability to perturb the systems we can play with the underlying interactions and make the best tests of theories.

In this thesis I will present measurements on two materials, the first Sr_2RuO_4 , known for its unconventional superconductivity, and the second $Sr_3Ru_2O_7$, for its quantum critical behaviour and large nematic-like susceptibility, and show how their properties can be manipulated through carefully applied uniaxial stress. Both materials are exquisitely clean, so to perturb them without destroying the fragile nature of Hamiltonian describing simple metals. \mathcal{H}_i describes the positive ion subsystem with masses M_i and charges Z_i . \mathbf{P}_i is the momentum of ion *i*. \mathcal{H}_e similarly describes the electron subsystem and \mathcal{H}_{e-i} accounts for the coulomb potential between the electrons and positive ions at positions \mathbf{r} and \mathbf{R} , respectively.

$$\mathcal{H} = \mathcal{H}_i + \mathcal{H}_e + \mathcal{H}_{e-i}$$
$$\mathcal{H}_i = \sum_i \frac{\mathbf{P}_i^2}{2M_i} + \frac{1}{2} \sum_{i \neq j} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$$
$$\mathcal{H}_e = \sum_i \frac{\mathbf{p}_i^2}{2m_e} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$
$$\mathcal{H}_{e-i} = -\sum_i \sum_j \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|}$$

the emergent phenomena a suitably clean tuning parameter is required. Significant technical development was needed to be able to apply a sufficiently homogeneous uniaxial pressure, so as well as the results a thorough discussion on the improvements to the technique that made this work possible will be given. Before this, though, I will start by briefly introducing how we describe the behaviour of electrons in metals, which will later form the basis for the specific discussions of each material presented in their respective chapters.

1.1 Electrons in Metals

To start the discussion of electron correlations in metals it is intuitive to begin with the free non-interacting case and then slowly introduce the correlations. In adopting this procedure, one must trust that reintroducing electron correlations later will not render the insights from the non-interacting case meaningless. In fact there are good reasons for this and a proper justification will be given in the section on Fermi liquids. Now also leaving the lattice of ions behind briefly, or better assuming a uniform positive background charge to maintain charge neutrality, we begin with the free Fermi gas and follow the Sommerfeld model. Conduction electron densities in metals are typically of the order 10^{22} cm⁻³ at room temperature [3]. At these densities the interparticle separations are less than the thermal de Broglie wavelength of the electrons. So to correctly describe the nature of this gas of electrons, quantum effects must be included and the electron gas will obey Fermi-Dirac statistics. Electrons occupy quantised energy states and obey the Pauli exclusion principle. Imagining a gas of electrons in a box of side *L* with periodic boundary conditions, the wavefunctions of the electrons are plane waves with energy

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m_e} \tag{1.1}$$



Fig. 1.1 Free electron Fermi surface. Each \mathbf{k} point within the sphere is occupied by one upand one down-spin electron

with quantised values of the wave-vector **k** in units of $(2\pi/L)$. The ground state is built up by filling up from the lowest energy state to the *N*th lowest state where *N* is the number of electrons. The highest occupied energy is called the Fermi energy $\varepsilon_{\rm F}$ with the corresponding Fermi wave-number $k_{\rm F}$. In reciprocal space the surface separating the volume containing all the filled states from the unoccupied states is called the Fermi surface, see Fig. 1.1 [3–5].

At non-zero temperature the population of states follows the Fermi-Dirac distribution. Thermal energy can excite an electron from within the filled Fermi surface to a state just outside creating an electron-hole pair. In a 'free electron metal' the typical Fermi temperature, $\varepsilon_F/k_B \sim 3 \times 10^4$ K, is much much higher than ambient temperature so only a small number of states within an energy of $\sim k_B T$ of the Fermi energy are ever excited. The Pauli exclusion principle prevents the excitation of the lower states since there are no unoccupied final states within $\sim k_B T$. This leads to a *T* linear specific heat, unlike the constant value for a classical gas, and a temperature independent magnetic susceptibility unlike the Curie-Weiss behaviour of the classical gas, both of which can be observed in real materials.

Reintroducing the periodic lattice, the wave-functions for the electrons are no longer plane waves but instead are described by Bloch waves [5]. The wave-vector or momentum used in the free electron picture no longer makes sense for the Bloch states because of the translational symmetry breaking. Instead, the electron states can be described by a quantity called crystal momentum.

The real space crystal structure is completely defined within the definition of the primitive unit cell. This irreducible volume can map out the whole structure by copying it along each of the translation vectors of the lattice. The same periodicity must exist in reciprocal space where the irreducible volume is now called the Brillouin zone. All momentum states can be mapped back to the first Brillouin zone through the reciprocal lattice vectors giving us the first idea of an electronic band structure, i.e. multiple bands of the electron dispersion, each at higher energy, within the first

1 Introduction



Fig. 1.2 Nearly-free electron dispersion. The free electron dispersion, dashed line, transforms into a set of discrete bands with energy gaps in between when a periodic potential with lattice constant *a* is weakly introduced

Brillouin zone. Each band has its own dispersion relationship, $E = E(\mathbf{k})$, but the number of possible states in each band is always equal to the number of allowed crystal momenta in the first Brillouin zone. This is always two times the number of primitive unit cells in the crystal, with the factor of two for spin degeneracy. Filling the allowed states proceeds as in the free electron gas and Sommerfeld model; starting from the lowest energy but now filling a new band when it is the next lowest in energy (Fig. 1.2).

Between each of the bands an energy gap develops, i.e. there are regions of energy where no Bloch wave solutions exist [4]. At wave-vectors satisfying the Bragg reflection condition of the lattice, the two left and right travelling wave-functions combine to form two different standing waves. The two standing waves have different probability densities, with one having higher probability at the lattice sites, and the other between lattice sites. There is therefore a difference in potential energy between the two solutions and this is the origin of the energy gap.

From the idea of Bloch waves we can extract a mean velocity for each of the electron states. At the Fermi energy we define the Fermi velocity

$$\upsilon_{\rm F} = \frac{1}{\hbar} \left. \nabla_{\mathbf{k}} \varepsilon \right|_{k_{\rm F}} \,, \tag{1.2}$$

and from this we can identity a band mass

$$m^* = \left(\frac{1}{\hbar^2 k_{\rm F}} \left. \nabla_{\mathbf{k}} \varepsilon \right|_{k_{\rm F}} \right)^{-1} \,. \tag{1.3}$$

This measures the impact of the lattice on the motion of the electrons by how much it differs from the bare electron mass m_e . We will see later that electron correlations can also enhance the effective mass further above the band mass.

When filling up states up to the Fermi level we can think of filling up to a surface with electrons but if only a few empty states remain close to the top of the band it is equally sensible to describe the band in terms of only the unoccupied states, or holes, at the top of the band. A hole is the absence of an electron so carries opposite charge and momenta to the electron states they are replacing.

There are two common limiting cases when continuing this discussion further; the periodic potential can be added to the free electron gas as a weak perturbation in a model called the nearly-free electron model, or we can start with atomic orbitals and slowly bring the lattice closer together allowing the electrons to hop between atomic sites described by the tight-binding model [5]. In this case, the itineracy is a perturbation on the atomic limit. The nearly-free electron model works very well for the alkali metals [5]. Although the Coulomb attraction to the lattice should at first sight be large, the Pauli exclusion principle keeps the conduction electrons in higher orbitals, further away from the ion cores on average, where the interaction is lower and the core electron model is entirely valid. For the alkali metals, with only one valence electron per atom, it is particularly good, because the Fermi surface fills only half of the first Brillouin zone, well away from the zone boundaries, thus avoiding the distortions of the band due to the band gaps [3].

For the materials we will be discussing later, Sr_2RuO_4 and $Sr_3Ru_2O_7$, both transition metal oxides, we are mainly concerned with the *d*-electron shell. For example, at the normal valencies for strontium and oxygen in Sr_2RuO_4 , Sr^{2+} and O^{2-} , the ruthenium ion with a valency of Ru^{4+} is left in a 4d⁴ electronic configuration [6]. The *d*-electron shells have small orbital radii meaning the interatomic overlap of the orbitals will be small and there will be a large potential penalty for double occupancy [7]. These factors take us away from the nearly-free electron limit. Many *d*-electron systems remain localized, forming a magnetic insulating state as opposed to a metallic one, especially in the 3d series [7]. The strontium ruthenate series is an exception and each remains metallic, but it is constructive to view them in a tight-binding fashion. I will now continue with a more formal description of the tight-binding model which will be useful for the derivations of the Fermi surfaces for both materials later.

In the tight-binding description we build the Bloch wavefunctions for the electrons from the atomic orbitals [3]. We assume the extent of the atomic orbitals, $\phi(\mathbf{r})$, is close to or smaller than the interatomic separation so they are mostly unperturbed when assembled into the lattice. The tight-binding wavefunction is a linear combination of approximately atomic orbitals [5]

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) \,. \tag{1.4}$$

The real space positions of the atoms determine how the bands develop. To illustrate this I will start with a simple cubic lattice, lattice constant a, of s states. We take a small perturbation, $V(\mathbf{r})$, to the atomic Hamiltonian which captures the periodicity of the lattice and look for the first-order corrections to the energy.¹

¹The wavefunctions are assumed to already be normalised here $\langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle = 1$.

1 Introduction

$$\Delta E = \langle \Psi_{\mathbf{k}} | V | \Psi_{\mathbf{k}} \rangle \tag{1.5}$$

$$=\sum_{n}\sum_{m}e^{i\mathbf{k}\cdot(\mathbf{R}_{n}-\mathbf{R}_{m})}\int\phi^{*}(\mathbf{r}-\mathbf{R}_{m})V\phi(\mathbf{r}-\mathbf{R}_{n})dV$$
(1.6)

$$=\sum_{m}e^{-i\mathbf{k}\cdot\mathbf{a}_{m}}\int\phi^{*}(\mathbf{r}-\mathbf{a}_{m})V\phi(\mathbf{r})dV$$
(1.7)

where $\mathbf{a}_m = \mathbf{R}_m - \mathbf{R}_n$. The integral is dominated by the on-site terms, $\mathbf{a}_m = 0$, and the six nearest neighbour terms, $\mathbf{a}_m = \pm a\hat{\mathbf{x}}, \pm a\hat{\mathbf{y}}, \pm a\hat{\mathbf{z}}$. We can drop all other terms because the atomic orbital overlap will be negligible. Thus we end up with

$$E(\mathbf{k}) = E_{\phi} - B - 2t(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)), \qquad (1.8)$$

where

$$B = -\int \phi^*(\mathbf{r}) V \phi(\mathbf{r}) dV \qquad (1.9)$$

$$t = -\int \phi^*(\mathbf{r} - \mathbf{a}) V \phi(\mathbf{r}) dV. \qquad (1.10)$$

The parameter t is known as the transfer integral, a measure of the ease of hopping from one atom to the next. In general, starting from n atomic levels on each atom, these will combine to form n separate bands. The bandwidth of the band is directly related to the transfer integral. A smaller atomic overlap, with a correspondingly smaller transfer integral, has a narrower bandwidth and a higher effective mass. In this way the effects of the real-space crystal structure are seen in the band structure; if in a certain direction the atoms are further apart, the bandwidth will be narrower for motion along that direction as is expected. The shape of the bands will also reflect the character of atomic orbitals they are made up from [5].

We have just seen two extreme cases for electrons in a metal; a scenario where the periodic potential is only a very weak perturbation to otherwise free electrons and the opposite extreme where the potential is so strong the electrons can hardly hop from one atom to the next. Both cases give rise to bands with corresponding gaps between them but crucially they are qualitatively similar. This implies that real materials, which will fall somewhere in between these two extremes, must also have qualitatively similar band structures.

1.2 Landau's Fermi Liquid

Up until now we have been ignoring the electron-electron Coulomb interaction but without foresight this should not have seemed like a sensible thing to do. By no means is the Coulomb interaction weak. Just making a quick back of the envelope calculation we can compare the scale of the Coulomb interaction with the kinetic energy of the electrons, which is the other important energy scale. From the electron density we can define a characteristic length, the radius of a sphere occupied by one electron, which sets the approximate kinetic energy $E_K \approx \hbar^2/8m_e r_s^2$ and the Coulomb repulsion between two electrons $E_C \approx e^2/8\pi\varepsilon_0 r_s$. The ratio gives us the importance of the electron-electron Coulomb interaction $E_C/E_K \approx r_s m_e e^2/\pi\varepsilon_0 \hbar^2 = 4r_s/a_0$, where a_0 is the Bohr radius. For typical metallic densities r_s is order Ångströms [3] whereas a_0 is half an Ångström. The electron-electron Coulomb interaction is not weak so how did we get on so well when we ignored it? The answer comes from Landau and his notion of a Fermi liquid [8–10]. If we start from a Fermi gas and turn on a mutual repulsion between all the electrons the Fermi gas turns into a Fermi liquid. The naming is in analogy to classical gases and liquids whereby introducing interparticle interactions condenses the gas to a liquid. The beauty is that the Fermi liquid retains some of the key properties of the Fermi gas.

By allowing the electrons to interact and exchange momentum the Fermi surface, in its original state, is no longer stable [11]. The insight of Landau was rather than caring about the individual electron states, to instead see what happens to the excitations of the Fermi gas as the electron-electron interaction is 'turned on'. An electron excited above the Fermi level can now Coulomb scatter with another below the Fermi level resulting in an additional electron-hole pair. This process can continue creating additional electron-hole pairs until some equilibrium is reached. This original excitation can now be described as the superposition of the bare electron, the bare electron and an electron-hole pair, the bare electron and two electron-hole pairs, and so forth [12].

$$|\Psi_{qp}\rangle = \sqrt{Z}|\phi_{el}\rangle + |\text{particle-hole excitations}\rangle + \dots$$
 (1.11)

The insight of Landau was that if we turn on the interaction slowly enough we can evolve smoothly from one picture to the other as the strength of the Coulomb interaction is increased. This concept is referred to as adiabatic continuity and we call the excited states of the interacting system Landau quasiparticles to remind us that the wavefunctions and energies are different from the corresponding electrons in the non-interacting problem. The quasiparticles do however retain the same charge and spin as the bare electron but neither the mass nor the interacting states with those of the non-interacting Fermi gas retains the picture of Fermi particles and a Fermi surface but one that is now stable since the Coulomb interaction has already been taken into account.

By producing the quasiparticles in this way they are made out of states which are no longer exact eigenstates of the system. Thus they cannot be infinitely long lived and the quasiparticles can scatter off one another. Their inverse lifetime can be calculated from Fermi's golden rule. Making reference to Fig. 1.3, a quasiparticle at energy ε scatters off one in the Fermi sea and looses energy ω . The total decay rate $1/\tau_{\varepsilon}$ for these processes is



Fig. 1.3 Quasiparticle scattering. A quasiparticle with energy ε above the Fermi surface can scatter off another from within the Fermi sea to create an additional particle-hole pair

$$\frac{1}{\tau_{\varepsilon}} = \frac{2\pi}{\hbar} \sum_{f} \left| V_{if} \right|^2 \delta(\varepsilon - \varepsilon_f)$$
(1.12)

where the sum is over all possible final states. We assume the scattering matrix elements $|V_{if}|$ are constant and make use of conservation of energy and momentum to restrict the possible final states. The Pauli exclusion principle also puts strict phase space restraints on the possible scatterings. There must be an unoccupied final state for the electron to scatter into so ω must be less than ε and the second electron must be within ω of the Fermi energy such that is can also reach an unoccupied state with the promotion of energy ω . Using the density of states at the Fermi level, g_F , to turn this into an integral

$$\frac{1}{\tau_{\varepsilon}} \sim \frac{2\pi}{\hbar} |V|^2 \int_0^{\varepsilon} g_{\rm F} d\omega \int_0^{\omega} g_{\rm F} d\varepsilon' \int_{-\infty}^{\infty} \delta(\varepsilon - \omega - \varepsilon' + \varepsilon'') g_{\rm F} d\varepsilon'' \tag{1.13}$$

$$\frac{1}{\tau_{\varepsilon}} \propto g_{\rm F}^3 \varepsilon^2. \tag{1.14}$$

We can now see that at sufficiently small energies close to the Fermi surface the quasiparticle is well defined. Here the quasiparticle's decay rate, $\propto \varepsilon^2$, is much less than its excitation energy ε . Further from the Fermi surface adiabatic continuity no longer holds, i.e. the quasiparticles scatter before the interaction can be completely turned on. Quasiparticles are therefore only well defined around the Fermi energy.

We are now in a position to see why the non-interacting case worked so well. The same phenomenology of electron-hole excitations from an electron Fermi sea applies for the Fermi liquid, but now the excitations are quasiparticle-quasihole excitations from the quasiparticle Fermi sea, and we recover the same qualitative predictions as those of the Sommerfeld model. Figure 1.4 shows how we can schematically think of this transformation. The electron probability distribution is modified under the presence of a weak mutual interaction but the sharp discontinuity at the Fermi wavevector survives. If instead we talk of the quasiparticles we recover the ordinary Fermi-Dirac distribution but as the quasiparticles are only well defined near the Fermi surface, we can only talk of small excitations from the Fermi energy.