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Contents

\mathbf{A}	Inte	raction effects in the electron gas	5
	A.1	Preamble: a model two-electron system	5
	A.2	Hartree approximation	7
	A.3	Hartree-Fock	7
	A.4	The homogeneous electron gas	9
в	Cha	rge Density Waves	13
	B.1	The Peierls transition	13
	B.2	Polyacetylene and solitons	17
	B.3	Semiclassical description	20
	B.4	Incommensurate density waves, sliding, and nonlinear dynamics .	21
С	The	Quantum Hall Effects	29
	C.1	Basic transport phenomena	29
	C.2	Landau level quantization	31
	C.3	Integer QHE	36
	C.4	Fractional QHE	38
D	Mag	gnetism	41
	D.1	Spin paramagnetism in metals	41
	D.2	Ferromagnetism in the Stoner-Hubbard model	42
	D.3	The origin of local magnetic moments	43
	D.4	Types of magnetic interactions	44
	D.5	Collective magnetic properties	48
		D.5.1 Magnetic phase transitions	48
		D.5.2 Spin waves	49

CONTENTS

D.5.3 Neutron scattering \ldots	 •	52
E Heavy fermions		55
E.1 The electron as a collective excitation		55
E.2 Local moments and the Kondo effect \ldots		58
E.3 Experimental properties of heavy fermion systems		60

Appendix A

Interaction effects in the electron gas

We have so far sidestepped entirely the effects of interactions between electrons, by working in the independent electron approximation with a one body potential $U(\mathbf{r})$ which somehow incorporates the interaction effects at the one particle level. Of course is clear that the *full* many-body Schrodinger equation cannot be described by a set of one-body equations. However, we can ask the question as to what is the *best* single particle representation, and independently we can ask how good it is. This will be the subject of this chapter.

If we fix the position of the ions, the electronic Hamiltonian is

$$H_{elec} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U_{ion}(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$
(A.1)

where the potential due to the ions is

$$U_{ion}(\mathbf{r}) = \sum_{I} \frac{Z_{I} e^{2}}{|\mathbf{r}_{i} - \mathbf{R}_{I}|}$$
(A.2)

where Z_I is the nuclear charge and \mathbf{R}_I the nuclear positions. We look for the solutions for the N-particle wavefunction $\Psi(\mathbf{r}_1, \sigma_1, ..., \mathbf{r}_N, \sigma_N)$ of the Schrödinger equation ¹

$$H_{elec}\Psi = E\Psi . \tag{A.3}$$

A.1 Preamble: a model two-electron system

The fundamental difficulty with treating interacting electronic systems is that we cannot expect to write a wavefunction that factorises into a product of

 $^{{}^{1}\}mathbf{r}_{i},\,\sigma_{i}$ are the space and spin coordinates of electron i

single electron wavefunctions. Such a factorisation is disallowed by the required antisymmetry of wavefunctions for fermions, namely that

$$\Psi(\mathbf{r}_1, \sigma_1, \dots, \mathbf{r}_i, \sigma_i, \dots, \mathbf{r}_j, \sigma_j, \dots, \mathbf{r}_N, \sigma_N) = -\Psi(\mathbf{r}_1, \sigma_1, \dots, \mathbf{r}_j, \sigma_j, \dots, \mathbf{r}_i, \sigma_i, \dots, \mathbf{r}_N, \sigma_N)$$
(A.4)

Here \mathbf{r}_i, σ_i are the position and spin of particle *i*, and fermion wavefunctions change sign when the coordinates of any two electrons are interchanged.²

Almost everything that we shall do on the interacting system can be understood in simple terms for a model of an atom (or a molecule) with two single particle orbitals and two electrons. We shall assume that the (orthonormal) single particle states $\psi_{1,2}(\mathbf{r})$ are unchanged by the interaction. There is an important simplification that arises also because the Coulomb interaction between particles is independent of their spin state, which we shall denote by $|\uparrow\rangle$, $|\downarrow\rangle$. In that case, we already know that the eigenstates of the two particle problem should be labelled by the total spin S and its z-component S_z . There will be four possible spin states

$$\begin{split} |\uparrow\uparrow\rangle & S_{z} = 1\\ \text{Triplet } S = 1 \quad (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} \quad S_{z} = 0\\ |\downarrow\downarrow\rangle & S_{z} = -1 \end{split} \tag{A.5}$$

Singlet
$$S = 0$$
 $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ $S_z = 0$ (A.6)

The notation is that $|\uparrow\downarrow\rangle = |\uparrow_1\rangle |\downarrow_2\rangle$, i.e. up spin for the electron labelled "1" and down spin for "2". The singlet state is *odd* under exchange of coordinates, and the triplet states are *even*. Because the total wavefunction must be odd, then the spatial wavefunctions that go along with these must be *odd* for the triplet states, and *even* for the singlet states. Since we decided at the outset that we are restricted to only two single particle states, we must have the following wavefunctions

$$\Psi_{T}(\mathbf{r}_{1}, \mathbf{r}_{2}) = (\psi_{1}(\mathbf{r}_{1})\psi_{2}(\mathbf{r}_{2}) - \psi_{2}(\mathbf{r}_{1})\psi_{1}(\mathbf{r}_{2}))/\sqrt{2}$$

$$= (|12 > -|21 >)/\sqrt{2}$$
(A.7)
$$\Psi_{S}(\mathbf{r}_{1}, \mathbf{r}_{2}) = (\psi_{1}(\mathbf{r}_{1})\psi_{2}(\mathbf{r}_{2}) + \psi_{2}(\mathbf{r}_{1})\psi_{1}(\mathbf{r}_{2}))/\sqrt{2}$$

$$= (|12 > +|21 >)/\sqrt{2} \tag{A.8}$$

where again we have used the notation that $|ij\rangle = \psi_i(\mathbf{r}_1)\psi_j(\mathbf{r}_2)$, so particle "1" is in the spatial wavefunction labelled by the state "i", and particle "2" is in state "j". The subscripts S and T label singlet and triplet wavefunctions, respectively.

Notice that the antiymmetry of the triplet wavefunction means that the electrons keep further apart than they would if they were independent distinguishable particles; in the singlet (symmetric) state they are closer together.

²Notice that the space and spin labels must both be interchanged.

A.2. HARTREE APPROXIMATION

This means that we expect that the triplet state is lower in energy than the singlet state, given the Coulomb repulsion. This can be shown explicitly using by evaluating the expectation value of the Hamiltonian using the two wavefunctions, which is

$$\langle H \rangle_{S,T} = E_1 + E_2 + \langle 12|V|12 \rangle \pm \langle 21|V|12 \rangle$$
, (A.9)

where the +/- signs are for singlet/triplet respectively. $E_{1,2}$ are the single particle energies - i.e. the expectation value of $T + U_{ion}$ - and the last two terms are matrix elements of the Coulomb interaction. The first of these is the direct, or Hartree energy

$$<12|V|12>=\int d\mathbf{r}d\mathbf{r}'|\psi_1(\mathbf{r}')|^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}|\psi_2(\mathbf{r})|^2$$
 (A.10)

which is just the interaction energy between the charge densities of the two electronic single particle states. The second of these has no analogue classically, and is called the exchange energy

$$<21|V|12>=\int d\mathbf{r}d\mathbf{r}'\psi_{2}^{*}(\mathbf{r})\psi_{1}^{*}(\mathbf{r}')\frac{e^{2}}{|\mathbf{r}-\mathbf{r}'|}\psi_{1}(\mathbf{r})\psi_{2}(\mathbf{r}')$$
 (A.11)

Despite the fact that the electron-electron interaction is independent of the spin of the electron, the requirement of antisymmetry of the wavefunction then produces a spin-dependent energy of the final state. This is the origin of magnetism in solids.

A.2 Hartree approximation

Returning to the many electron problem, we can now repeat the calculation more formally, but this time not restricting the single particle basis to predetermined states. The most natural first approximation to the difficult interaction term in Eq. (A.1) is to replace the interaction between the electrons by a set of interactions between a single electron and the charge density made up from all the other electrons, i.e. by a one-body potential for the i^{th} electron

$$U_{coul}(\mathbf{r}) = -e \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{\mathbf{r} - \mathbf{r}'} = e^2 \sum_{j \neq i} \int d\mathbf{r}' \frac{|\psi_j(\mathbf{r}')|^2}{\mathbf{r} - \mathbf{r}'} , \qquad (A.12)$$

where the summation is over all the occupied states ψ_i . This clearly takes into account the averaged effect of the Coulomb repulsion due to all the other electron, and corresponds to the term Eq. (A.10) above.

A.3 Hartree-Fock

One of the primary deficiencies of the Hartree approximation is that the wavefunctions violate the Pauli principle. This was precisely the physics that we were at pains to incorporate in the model two-electron problem above. The simplest wavefunction that satisfies this requirement is the *Slater determinant*

$$\Psi_{HF} = \begin{vmatrix} \psi_1(\mathbf{r}_1, \sigma_1) & \cdots & \psi_1(\mathbf{r}_N, \sigma_N) \\ \vdots & \vdots \\ \psi_N(\mathbf{r}_1, \sigma_1) & \cdots & \psi_N(\mathbf{r}_N, \sigma_N) \end{vmatrix} .$$
(A.13)

Hartree-Fock theory is formally defined as the *best* (in a variational sense) single Slater determinant — i.e. which involves finding the "single particle" basis states ψ_i . We won't need this in order to do study a homogeneous system, because in that case the states are determined by symmetry to be *plane waves*. But here is the general analysis.

If one evaluates the energy in the form

$$< H >_{\Psi} = \frac{<\Psi|H|\Psi>}{<\Psi|\Psi>}$$

with the determinantal wavefunction of Eq. (A.13) using an orthonormal set of orbitals ψ_i , one gets ³:

$$< H >_{\Psi} = \sum_{i} < i |(T + U_{ion}|i) > + \frac{1}{2} \sum_{ij} \left[< ij |\frac{e^2}{r_{ij}}|ij\rangle - < ij |\frac{e^2}{r_{ij}}|ji\rangle \delta_{\sigma_i \sigma_j} \right] .$$
(A.14)

(This calculation is much trickier than it looks).

Then one can variationally minimise with respect to the ψ_i^* obtaining the Hartree-Fock equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ion}(\mathbf{r}) + U_{coul}(\mathbf{r})\right]\psi_i(\mathbf{r}) - \sum_j \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')\psi_j(\mathbf{r})\delta_{\sigma_i\sigma_j} = \epsilon_i\psi_i(\mathbf{r})$$
(A.15)

After solving Eq. (A.15) to determine the wavefunctions and the energy eigenvalues the total energy can be written 4

$$\langle H \rangle_{\Psi} = \sum_{i} \epsilon_{i} - \frac{1}{2} \sum_{ij} \left[\langle ij | \frac{e^{2}}{r_{ij}} | ij \rangle - \langle ij | \frac{e^{2}}{r_{ij}} | ji \rangle \delta_{\sigma_{i}\sigma_{j}} \right] .$$
(A.16)

The equations are similar to the Hartree equations, but have an extra term, the *exchange* term which is not only nonlinear in ψ but also *non-local*, and *spin-dependent*. Such complexity makes them very difficult to solve in practice.

Thus when we draw a band-structure in the independent particle approximation, at the Hartree-Fock level that corresponds to the variation energies ϵ_i , of Eq. (A.15); the corresponding many-body wavefunction is then the Slater-determinant obtained by entering the lowest energy eigenstates into the determinant Eq. (A.13). Notice that if we have a system that is a paramagnet, there will be two degenerate eigenstates for each spin. The exchange energy lowering (note the sign) only occurs between states of the same spin (i.e. half the pairs in a paramagnet).

³We shall use the notation $\langle i|f|j \rangle = \int d\mathbf{r} \, \phi_i^*(\mathbf{r}) f(\mathbf{r}) \phi_j(\mathbf{r})$ for one body matrix elements, and $\langle ij|f|mn \rangle = \int \int d\mathbf{r} \, d\mathbf{r}' \, \phi_i^*(\mathbf{r}) \phi_j^*(\mathbf{r}') f(\mathbf{r},\mathbf{r}') \phi_m(\mathbf{r}) \phi_n(\mathbf{r}')$ for two-body matrix elements.

⁴Notice that this is not equal to the sum of single-particle energies, because otherwise the interaction terms would be counted twice

A.4 The homogeneous electron gas

The one case where the Hartree-Fock equations can be solved straightforwardly is the not uninteresting case of *jellium*: the periodic lattice potential is replaced by a uniform positive background that neutralises the electronic charge. Owing to translational symmetry, the single particle states in the Slater determinant must be plane waves:

$$\psi_i(\mathbf{r}) = (V)^{-\frac{1}{2}} e^{i\mathbf{k}_i \cdot \mathbf{r}} \times \chi_{spin} \tag{A.17}$$

where we occupy each wavevector $|\mathbf{k}| < k_F$ twice (once for each spin component). One can evaluate the Hartree-Fock energy without having to solve for the wavefunctions, which is the hard bit in a problem on a lattice.

Units

It is useful at this point to introduce the electron gas density parameter r_s .

• Since the energy scale is set by the Coulomb potential, it is convenient to measure energies in units of the Rydberg:

$$1Rydberg = \frac{\hbar^2}{2ma_B^2} = \frac{e^2}{8\pi\epsilon_0 a_B} \quad , \tag{A.18}$$

with a_B the Bohr radius.

• Then we measure the density n in units of the Bohr radius by

$$4\pi (r_s a_B)^3 / 3 = 1/n \tag{A.19}$$

so r_s is a dimensionless parameter, which is the average spacing between electrons measured in units of the Bohr radius.

• In a medium where the electrons have an effective mass m^* , and there is a background relative dielectric constant ϵ , then there is an effective Bohr radius

$$a^* = \epsilon \frac{m^*}{m} a_B \tag{A.20}$$

and an effective rydberg

$$Ry^* = \frac{1}{\epsilon^2} \frac{m^*}{m} Ry \tag{A.21}$$

For electrons in the semiconductor GaAs, $\frac{m^*}{m} \approx 0.1$ and $\epsilon \approx 13$, so $a^* \approx 7$ nm and $Ry^* \approx 5$ meV

10 APPENDIX A. INTERACTION EFFECTS IN THE ELECTRON GAS

Evaluation of the exchange energy

The energy can be evaluated as follows. The direct Coulomb energy cancels exactly with the ionic energy: $U_{Coul} + U_{ion} = 0$. We are left with only the kinetic energy and the exchange energy. The kinetic energy term in Eq. (A.15) gives

$$-\frac{\hbar^2}{2m}\nabla^2 e^{i\mathbf{k}_i\cdot\mathbf{r}} = \frac{\hbar^2 k^2}{2m} e^{i\mathbf{k}\cdot\mathbf{r}}$$
(A.22)

and the exchange term in Eq. (A.15) becomes

$$U_{exch}V^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}} = -\sum_{|\mathbf{q}| < k_F} V^{-\frac{1}{2}}e^{i\mathbf{q}\cdot\mathbf{r}} \int d\mathbf{r}' V^{-\frac{1}{2}}e^{-i\mathbf{q}\cdot\mathbf{r}'} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} V^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}'}$$
$$= -(V)^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}} \times \frac{1}{V} \sum_{q < k_F} \int d\mathbf{r}' e^{-i(\mathbf{k}-\mathbf{q})\cdot(\mathbf{r}-\mathbf{r}')} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}$$
$$= -(V)^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}} \times \frac{1}{V} \sum_{q < k_F} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{q}|^2} .$$
(A.23)

Eq. (A.23) makes use of the familiar result that the Fourier transform of the Coulomb potential 1/r is just $4\pi/q^2$.

The energy can be evaluated in closed form

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} - \int_{k' < k_F} \frac{d\mathbf{k}'}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{k} - \mathbf{k}'|^2} = \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} F(k/k_F) , \qquad (A.24)$$

where

$$F(x) = \frac{1}{2} + \frac{1 - x^2}{4x} \ln \left| \frac{1 + x}{1 - x} \right| .$$
 (A.25)

The total energy can be performed by integration over $k < k_F$ It is ⁵

$$E_{tot}^{HF} = 2 \sum_{k < k_F} \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} \sum_{k < k_F} F(k/k_F)$$

= $N \left[\frac{3}{5} \frac{\hbar^2 k_F^2}{2m} - \frac{3}{4} \frac{e^2 k_F}{\pi} \right]$ (A.26)

This result is conventionally written in rydberg units, using the electron gas density parameter r_s (Eq. (A.19)) as

$$E_{tot}^{HF}/N = 2.21r_s^{-2} - 0.916r_s^{-1} \tag{A.27}$$

For a typical metal r_s is in the range of 2-4, and the second term is comparable in size to the first.

The first term in Eq. (A.27) is from the kinetic energy, and the second from the exchange interactions (the Hartree term is exactly cancelled by the

⁵Notice a factor of two for spin, and a factor of 1/2 (double-counting) in the second term

interaction with the postive background). The kinetic energy term is the larger at smaller r_s , which means higher density - despite the electrons coming closer to each other. This is of course precisely the opposite result that one would have got for a classical gas (where the "perfect gas" limit is the *dilute* limit. The difference is because electrons are fermions, and as one goes to higher density, the Fermi energy E_F increases more rapidly than the interaction energy. *High density metals are free-electron like*.

Eq. (A.27) looks like the first few terms in a series expansion starting from the high density limit. The series continues⁶

$$E_{tot}/N = 2.21r_s^{-2} - 0.916r_s^{-1} + 0.0622\ln(r_s) - 0.096 + O(r_s) + \dots$$
(A.28)

The difference in energy between the exact energy and the Hartree-Fock energy is often termed the *correlation energy*.

Ferromagnetic liquid

Remember that the exchange energy lowering was only between parallel spins, and therefore came in to only half the terms in the exchange energy. In a spinaligned (ferromagnetic) ground state wave-function, then the exchange energy (lowering) will be larger - twice as many terms. However the kinetic energy (positive) will also be larger because there will be a larger k_F (by a factor of $2^{1/3}$) if only one spin subband is filled. The interaction terms become proportionately more important at low densities (large r_s) than the kinetic energy, so we may expect that the dilute electron gas is ferromagnetic.

Qu.1.1 Ferromagnetism in the HF approximation

Consider a fully spin polarised state: the Hartree-Fock Slater determinant corresponds to singly occupying each state in the Fermi sphere. In analogy to Eq. (A.26), compute the total energy of the spin polarised state, and show that this is lower in energy than the unpolarised state if $r_s > 5.45$ in the Hartree-Fock approximation. The physics here is correct, but the numerical answer very wrong — the paramagnetic state is believed to be stable up to $r_s \approx 75$.

Wigner crystal

Interactions become relatively more important as the density decreases, because the kinetic energy penalty for keeping electrons apart is reduced. But we are still describing the electrons as a fluid, albeit a quantum fluid; our experience tells us that if repulsive interactions get large enough, the ground state of the system

⁶Gell-Mann and Brueckner, Phys. Rev. 106, 364 (1957).

should not be a fluid but a solid. Quite some time ago, Wigner⁷ argued that the electron gas must crystallise at low enough density. The argument is quite simple, but quite beyond the reach of the independent electron approximation.

In an electron solid, each electron is assumed to be localised to a site on a lattice, not spread out through the crystal as in the metallic state we have been discussing hitherto. If the electrons are well localised and only weakly overlap with each other, one can estimate the energy quite simply.

The Coulomb energy is just the energy of interacting charged particles - the Hartree term. If you include the Jellium background, the interaction of with the N-1 other electrons is approximately cancelled by their counterbalancing background charge. What remains is the Coulomb energy of a single electron that has a uniformly charged sphere of jellium around it. This is of order

$$-\frac{e^2}{2a_B r_s} \tag{A.29}$$

(One can improve the estimate by doing the calculation summing over all the charges; this multiplies the result by a factor of α , called a Madelung constant. Generally $\alpha \approx 1.7$ depending on the crystal lattice structure).

The kinetic energy cost of localising the electron is just the zero point energy of localising the electron inside the sphere which should be of order

$$\frac{\hbar^2}{2ma_B^2 r_s^2} \tag{A.30}$$

Thus we estimate

$$E_{tot}^{WC}/N \approx -\frac{1}{2}\alpha r_s^{-1} + r_s^{-2} Ryd.$$
 (A.31)

For large enough r_s , the coulomb energy must always win – because asymptotically the dominant energy term is negative, and scales as $r_s^{-1.8}$ Comparing Eq. (A.31) with Eq. (A.28) suggests a transition near $r_s \approx 5$, whereas the best calculations place it closer to $100.^9$

⁷E.P.Wigner, *Phys. Rev.* **46**, 1002 (1934)

⁸Notice that Eq. (A.31) is an expansion in powers of $(1/r_s)$ about the *low*- density limit $(r_s \to \infty)$, whereas Eq. (A.28) is an expansion in powers of r_s about the *high*-density limit $(r_s \to 0)$.

⁹The most reliable estimates come from quantum Monte Carlo calculations, see D.Ceperley and B.J.Alder, *Phys. Rev. Lett.* **45**, 566 (1980).

Appendix B

Charge Density Waves

The crystal structures of solids are much more complex than one might have expected. Even if you take the elements, rather few form simple close-packed structures. For example Ga metal has a complicated structure with 5 nearest neighbours, Se crystallises in a structure that can be thought of as an array of spiral chains with three atoms per unit cell, As, Sb and Bi have puckered sheets where each atom has three near neighbours.

Of course, all of this reflects the production of chemical bonds inside the solid, and a complicated balance of forces. But the fundamental principle of bonding is that by placing the chemical potential in a gap, the occupied states are lowered in energy (and the unoccupied states go up in energy). Getting the chemical potential to lie in a gap involves making sure that the Brillouin zone boundary lies "in the right place", i.e. at a momentum that will contain exactly the correct number of states to account for all of the electrons in the solid.

B.1 The Peierls transition

As a concrete example we consider a one-dimensional chain of atoms, with lattice constant a, and an electron density chosen such that the fermi wave-vector k_F falls somewhere in the middle of the band. It is a metal.

Notice that we could turn this metal into an insulator by applying an *external* potential with a periodicity of $2\pi/Q$ where $Q = 2k_F$: following the earlier lectures, we know that a periodic potential $V_o \cos(Qx)$ produces Bragg scattering at a wavevector Q/2 (hence a new Brillouin zone boundary). If $Q/2 = k_F$ then there is a gap induced on the fermi surface.

Rather than applying an external potential, we could get the same effect by making a periodic lattice distortion (PLD) with the same periodicity: namely



Figure B.1: The Peierls transition. The upper figure shows the familiar onedimensional chain with lattice constant a and the corresponding lowest electronic band, plotted for momenta between 0 and π/a . In the lower figure (b) a periodic lattice modulation is introduced, with u(r) of the form of Eq. (B.1). The period is cunningly chosen to be exactly $2\pi/2k_F$, so that a band gap of amplitude $2g_Q u_0$ is introduced exactly at the chemical potential.

move the n^{th} atom in the chain to a new position

$$R_n = na + u_o cos(Qna) \quad . \tag{B.1}$$

We assume that the amplitude of the PLD is small, $u_o \ll a$. [We have already met this phenomenon in the diatomic chain, studied earlier, but where we considered the case of a half-filled band — in that case $k_F = \pi/2a$ and $Q = \pi/a$, and the periodicity of the distorted lattice is twice that of the undistorted one.]

If the atoms have a PLD with period $2\pi/Q$, they will produce a new potential seen by the electrons with the same period. It is also evident that the amplitude of the Fourier component $V_Q \propto u_o$ is linearly proportional to the displacement (for small displacements). We may write $V_Q = g_Q u_o$, where the coefficient g_Q is the electron-phonon coupling constant.

Now remember that the energy gap on the zone boundary is $|V_Q|$. That means that an energy level at a momentum just below k_F is lowered by an energy proportional to the atomic displacement $|u_o|$, (and the unoccupied one just above k_F is raised in energy by the same amount). So overall there is an energy lowering as a result of the PLD. The magnitude of this can be computed (see the problem below) by adding up all the energy changes of all occupied states: the answer can be written as

$$E_{electronic} = A(u_o/a)^2 \ln |u_o/a| \tag{B.2}$$

in the limit $u_o/a \ll 1$, and A is a constant (depending on g_Q). Note the logarithm — this varies faster than quadratically (just). It is negative - the energy goes down with the distortion.

By an extension of the standard band structure result, it should be clear that there is an electronic charge modulation accompanying the periodic lattice distortion - this is usually called a charge density wave (CDW).

Eq. (B.2) is just the electronic contribution to the energy from those states very close to the fermi surface. But as we have argued before, it is sensible to model the other interactions between atoms just as springs, in which case we should add an elastic energy that is of the form

$$E_{elastic} = K(u_o/a)^2 \tag{B.3}$$

Adding the two terms together gives a potential of the form

$$E(x) = Ax^2 \ln|x| + Bx^2 \tag{B.4}$$

which *always* has a minimum at non-zero displacement. The system lowers its energy by distorting to produce a PLD and accompanying CDW, with a period that is determined by the fermi wave-vector, viz. $2\pi/2k_F$. Such a spontaneous lattice distortion is a broken symmetry phase transition (see Fig. B.2), that goes by the name of its discoverer, Peierls. It tells us that a one-dimensional metal is always unstable to the formation of a CDW, even if the electron-phonon coupling is weak. $^{\rm 1}$

Qu.2.2 *Peierls transition in a one-dimensional electronic band

Consider a one-dimensional system which is filled up to the first Brillouin zone boundary at $k = \pi/a$, and assume that there is a small gap produced by a single Fourier component of the lattice potential $U = U_{K=2\pi/a}$ (small meaning that $U/E_{\frac{1}{2}K}^0 \ll 1$). Consider momenta close to the zone boundary, show that a good approximation for the energy dispersion of the bands is

$$E = E_0 \left(1 \pm \sqrt{\frac{U^2}{E_0^2} + 4\kappa^2} \right)$$

where $E_0 = E_{\frac{1}{2}K}^0$ and $k = (\pi/a)(1+\kappa)$, with $\kappa \ll 1$.

Show that the change in electronic energy

$$E_{elec} = \frac{1}{N} \sum_{k \text{ occupied}} \left[E(k; U_K) - E(k; U_K = 0) \right]$$

can be written approximately as

$$E_{elec} = 2|U| \int_0^1 dx \left[\frac{x}{\alpha} - (1 + \frac{x^2}{\alpha^2})^{1/2}\right] \propto \frac{\hbar^2 \pi^2}{ma^2} \alpha^2 \log(\alpha) \quad ,$$

in the limit that the parameter $\alpha = \frac{ma^2}{\hbar^2 \pi^2} |U|$ is much smaller than unity (i.e. the gap is small compared to the bandwidth.

Materials that are strongly anisotropic in their electronic structure are thus prone to a spontaneous lattice distortion and accompanying charge density wave. (The logarithmic singularity does not appear in dimensions greater than one although CDW's indeed happen in higher dimension, they don't necessarily occur in weak coupling).

Commonly there will be a phase transition on lowering the temperature that corresponds to the onset of order — one can monitor this by the appearance of new Bragg peaks in the crystal structure, seen by electron, neutron, or X-ray scattering (see Fig. B.3).

¹There are of course other periodicities produced by beating of the spatial frequencies Q with $2\pi/a$. These need not concern us if the amplitude is small, because they will generally occur at momenta different from k_F , so the gap will lower and raise the energy of pairs of states that are either both unoccupied or both occupied, cancelling in the total energy.



Figure B.2: Sketch of Eq. (B.4) showing the double minimum of energy

More subtly, the onset of a CDW can be seen in the phonon spectrum. Notice that by calculating the energy change as a result of a small lattice displacement, we have in the coefficient of the quadratic term in the energy as a function of displacement, the phonon stiffness for a mode of the wavevector $2k_F$. Consequently, the onset of a CDW is when the stiffness becomes *zero* (and negative below the transition), so there is no restoring force associated with the displacement. Then the phonon spectrum $\omega(q)$ (even in the high temperature undistorted phase) will be expected to show a sharp minimum in the vicinity of $q = 2k_F$, as seen in Fig. B.4.

B.2 Polyacetylene and solitons

One of the celebrated cases of such a CDW occurs in the polymer $(CH)^n$, transpolyacetylene (Fig. B.5). Of the 4 valence electrons contributed by each carbon atom, one is involved in a bonding band (non-dispersive) with the H, leaving 3 electrons per atom to be accommodated along the -C - C - C - chain. If the C atoms were equally spaced, then there would be one full and one half-filled band. This half-filled band is unstable to dimerisation by the Peierls mechanism — doubling the lattice period, halves the Brillouin zone. It is often idealised as an alternation of double and single bonds, viz. -C = C - C - C - c.

The figure Fig. B.5 shows that there are two different but symmetry-related ground states that can be formed by the dimerisation. One can readily imagine that in a long chain, these two states might join up next to each other, and that situation is visualised in Fig. B.6. The boundary between the two regions cannot be locally "unwound", because a large number of atoms will have to be



Figure B.3: Electron diffraction image shows Bragg scattering from a CDW formed in the compound $La_{0.29}Ca_{0.71}MnO_3$. The real space image is at the top, showing a short scale checkerboard that is the atomic lattice, with a periodic modulation. The bottom figure is the fourier transform, so that the widely spaced bright peaks come from the small unit cell (this compound is based on a cubic perovskite, where the Mn atoms are on a simple cubic lattice), and the less intense peaks in between are the CDW. The two periods (lattice and CDW) are not related, because the CDW period is determined by the fermi surface size and shape, which depends on the electron concentration. Here the presence of an incommensurate ratio of trivalent La to divalent Ca means that the Mn d-bands are only partially filled. [Image courtesy of J. Loudon, P.A. Midgley, N.D. Mathur]



Figure B.4: Phonon dispersion curves in the quasi- one-dimensional organic compound TTF-TCNQ (tetrathiofulvalene tetracyanoquinone) along the direction of the chains in which there is a prominent soft phonon that turns into a periodic lattice distortion at low temperature. (There are many non-dispersing optical modes in the complicated unit cell.)[Mook and Watson, Phys. Rev. Lett. **36**, 801 (1976)]



Figure B.5: (a) shows a sketch of the atomic arrangement of polyacetylene, with the C atoms as solid circles, and the H atoms as open circles. The C atoms are not equally spaced, and the structure is often idealised as an alternation of "double" and "single" bonds, (b) and (c). The two isomers in (b) and (c) are related by a mirror symmetry.



Figure B.6: In (a) we create a region of dimerisation of the opposite sign in the middle of another domain. The boundaries between the regions are "solitons" (that are in practice several lattice constants wide), and one can see from the schematic arrows that they are charged. (b) These are often described using a phase degree of freedom, Eq. (B.5), which is sensible provided the variation is slow (as it often is). The solitons act as potentials that can trap either electrons or hole (c), producing new kinds of quasiparticles that have the spin of the carrier but are electrically neutral.

displaced to do so. There is a topological distinction between the two states.

B.3 Semiclassical description

The *solitons* that form the boundaries are similar in character to a domain wall in a magnet, (there separating a homogeneous region of spin-up from spindown). A convenient semiclassical description is to write the modulated CDW as

$$\rho(\mathbf{r}) = \rho_c + \rho_o \cos(\mathbf{Q} \cdot \mathbf{r} + \phi(\mathbf{r})) \quad , \tag{B.5}$$

where the CDW is described by an amplitude ρ_o and a phase $\phi(\mathbf{r})$. ρ_c is the (uniform) background density of the electron gas. If the phase is a constant, it just defines the alignment of the density wave relative to the underlying lattice - and in the case of polyacetylene, the two states (b) and (c) of Fig. B.5 are described by phases different by exactly π .

In the solitonic domain wall, the phase is smoothly modulated between the two minima - the CDW is expected to be elastic so that its period will not change abruptly. In a coarse-grained semiclassical theory for the CDW, one expects that the Hamiltonian density can be expressed to leading order just as a function of the phase alone, viz.

$$H = \int dx \left[\frac{1}{2} K \left(\frac{\partial \phi}{\partial x} \right)^2 - V_c \cos(2\phi) \right] \quad , \tag{B.6}$$

The first term in Eq. (B.6) is just the elastic energy cost of stretching or compressing the CDW, and the second term is the *commensurability* energy, which favours $\phi = 0, \pi$ as the two broken symmetry ground states.

We can extract from this the equation to describe a soliton from the variational minimisation of Eq. (B.6)

$$K\frac{d^2\phi}{dx^2} = 2V_c\sin(2\phi) \tag{B.7}$$

which integrates up to an elliptic integral. The width of the soliton is proportional to $(K/V_c)^{1/2}$, as can be seen using dimensional arguments from the above. In polyacetylene, the soliton width is believed to be about 10 lattice constants, large enough to justify the coarse-graining procedure above.

In the figure above, I indicated that the soliton boundary is charged, and let us now make that argument a bit more solid. The CDW in equilibrium is expected to have $Q = 2k_F$ to minimise the energy by putting a gap at the fermi surface. However, suppose the wavevector shifted locally to $Q + \delta Q$, where using Eq. (B.5) we have $\delta Q = \nabla \phi(r)$.

Of course this puts a gap in " the wrong place", and if this were the case everywhere in the solid, the chemical potential will lie in a band and the material is a metal. But consider the situation where a local increase in δQ is balanced elsewhere by a decrease. In some regions of the sample, the positive δQ makes holes; elsewhere, a negative δQ generates electrons. This is a situation that is not in equilibrium, because it would require a different chemical potential in the different regions of the sample: after the potential has reached equilibrium, there will be a net charge flow to make the chemical potential lie everywhere in a gap (Fig. B.7). By counting the states that have been filled, one gets for a physical charge density

$$\rho = -\frac{e}{\pi}\delta Q = -\frac{e}{\pi}\nabla\phi \tag{B.8}$$

The charge contained in the polyacetylene domain wall is exactly $\pm e$, as advertised.

This is no more than saying that when one compressed the CDW, one compresses not only the wave, but the *whole* of the electron density - see Fig. B.7.

B.4 Incommensurate density waves, sliding, and nonlinear dynamics

Polyacetylene is a simple case where the CDW is commensurate with the underlying lattice - a doubling of periodicity. Here there are two inequivalent states,



Figure B.7: In (a) the CDW is compressed (larger local wavevector) so the gap occurs at a wavevector greater than k_F . Elsewhere in the solid, it may be extended, as in (b). In order to keep chemical equilibrium between these two regimes, there is charge flow from one region to the other, and overall the chemical potential stays in the energy gap. The arrangement of the charge density in real space is shown in (a') and (b') below, stressing that the whole charge density is modulated, including ρ_c .



Figure B.8: Dark field image of the charge-density wave order in $TaSe_2$. The dark lines mark domain walls in the CDW; notice that they occasionally join together in threes. See C. H. Chen, J. M. Gibson, and R. M. Fleming Phys. Rev. B 26, 184-205 (1982), which also gives a detailed explanation of the methodology of dark-field imaging of CDW. The origin of contrast here is in fact rather special to the internal structure of the commensurate phase, but makes for some striking pictures

and the charge on the domain wall is 2e/2. Fig. B.8 shows images of domain walls in the two-dimensional material $2H - TaSe_2$, which is nearly period 3 (i.e. Q = G/3, where G is a reciprocal lattice vector of the undistorted lattice). In this case, there are three different (but identical in energy) topological states — the domain walls have charge 2e/3 per unit cell — and the domain walls can combine in three only at a vortex like defect.

Depending on the chemistry of the material, we may have CDW's that are entirely incommensurate with the underlying lattice, meaning that the periods bear no rational relationship. Notice that this means that the broken symmetry is now continuous - i.e. any value of the phase ϕ is equally good.

This is interesting — since $\nabla \phi$ is a charge, ϕ itself is a polarisation. This means that an electric field **E** will couple to the *phase* of the CDW, with an energy $\mathbf{P} \cdot \mathbf{E} = (e/\pi)\phi E$, picking out the component of the electric field in the direction of **Q**. An electric field therefore exerts a force on the CDW.

What is there to hold the CDW back? If the CDW is uniform, its energy does not depend on where it sits, but in a real solid there are always defects and impurities pin the CDW by locally deforming it. This means that a finite field has to be applied before the CDW will move, but beyond this threshold field the whole CDW slides through the lattice, reaching an equilibrium velocity determined by the "frictional force" induced by the relative motion with the underlying lattice. Because the CDW is rather stiff, it is not easy to pin, and



Figure B.9: The inset shows the current induced in the cdw material TaS_3 , and the main panel is the differential conductance $\sigma = dI/dV$. Below a threshold voltage, the CDW is pinned, and the only contribution to the current is the thermal activation of carriers across the CDW gap. Above V_T , there is a large contribution to the current that grows in a nonlinear fashion with increasing voltage, which is the contribution of the sliding of the CDW.[From Gruner and Gorkov,]

the electrical fields required to get it to move can be small - no more than Vm^{-1} in some cases.

This physical system has turned out to be an interesting fruit fly to study the nonlinear dynamics of extended, dissipative systems. We will just exhibit a few examples of phenomena.

Non-linear I-V characteristics. Above a threshold field E_T , the current grows in a non-linear fashion, $I \propto (E - E_T)^{\nu}$. It turns out that this is a true dynamic critical phenomenon - just as at a phase transition with temperature an order parameter turns on in a non-analytic fashion, so here the CDW current plays the role of the order parameter (Fig. B.9).

AC Noise. When the CDW is moving, at any point the CDW is sliding past the pinning sites like a washboard. As it moves past, it undergoes a periodic stick-slip motion, being periodically held back and then released. This means that in consequence, the motion is not purely DC, but has an AC component whose frequency is proportional to the DC current(Fig. B.10). If one applies both an AC and a DC electric field, one can observe complex nonlinear dynamics where the internal and external frequencies can be locked together (Fig. B.11).

Giant dielectric constant. Below threshold, while an electric field is not enough to induce a steady current, it can produce a very large polarisation by



Figure B.10: The output of a spectrum analyser of a sliding CDW system shows peaks at frequencies (and their harmonics) that increase with increasing cdw current. Measurements of the DC current show that the frequencies of the narrow band noise peaks are consistent with the "washboard" motion: namely $\omega_{noise} \approx Qv$, with $v = j_{CDW}/ne$ the CDW velocity, inferred from the measured current j_{CDW} and density n. The different curves are measured with increasing dc current, from below threshold (e) - no sharp peaks - to the highest velocity (a). [From Gruner and Gorkov]



Figure B.11: Here the CDW is driven by both a DC and AC field $V(t) = V + V_{RF} \cos(\omega_{RF}t)$. Plotted is the resistance dV/dI for difference magnitudes of V_{RF} . The top curve is just the non-linear threshold behaviour, as seen above (Fig. B.9), and the constant below threshold is just the resistivity of single particles (it turns out that $NbSe_3$ is a metal, so this is small. In the presence of the RF field, new plateaus appear, corresponding to mode-locking of the CDW when the washboard frequency is a rational multiple of the driving frequency - often called a "devil's staircase".

deforming the CDW over large distances (Fig. B.12.)

Glassyness. The state below threshold is not unique, and is a model glass which has barriers of varying sizes. This means that it has a distribution of oscillation modes so that the response is not the Lorentzian of a single damped oscillator, but has power law tails down to arbitrarilylow frequencies.

Avalanches. If you increase the field below threshold, larger and larger pieces of the CDW try to break free, producing avalanches of increasing size as threshold is approached. In fact CDW systems are nice models in the lab for earthquake dynamics, and so-called "self-organized criticality" (Fig. B.13).

Further reading

G. Gruner, "Density Waves in Solids", Addison-Wesley Publishing Company, 1994.



Figure B.12: Real and imaginary parts of the dielectric response function $\epsilon(\omega)$ of the material $K_{0.3}MoO_3$, which has a charge density wave below 180 K. A typical dielectric material like a semiconductor has a dielectric constant of order 10 at most; and the frequency dependence occurs on the scale of the electronic transitions. A CDW behaves like a sluggish (frequency dependence on the kHz to MHz scales) and highly polarisable (static dielectric constants up to 10^7) medium. [Cava et al. Phys. Rev. B **30**, 3228 (1984)]



Figure B.13: Real part of the dielectric response function $\epsilon(\omega)$ in $K_{0.3}MoO_3$, as a function of d.c. bias. As the electric field increases towards threshold, the medium becomes more an more polarisable, until at threshold the linear response diverges. The resonant features above threshold occur when the driving frequency matches the internal "washboard" of the moving CDW. [Cava et al. *ibid*]

Appendix C

The Quantum Hall Effects

C.1 Basic transport phenomena

The quantum Hall effects are a set of phenomena observed at low temperatures in very high mobility electron gases in two dimensions, in the presence of a perpendicular magnetic field.

The basic phenomena are the discovery that the Hall conductance of the system has integer quantisation in terms of the fundamental unit $e^2/h \approx (26 \ k\Omega)^{-1}$ by von Klitzing, Dorda and Pepper in 1980. In 1982 Tsui, Stormer and Gossard found that at lower temperatures in samples that have higher mobilities, the Hall conductance can be a rational fraction of e^2/h .

Heterostructures and the 2D electron gas.

We discussed earlier the technique of modulation doping to produce a twodimensional electron gas in a semiconductor heterostructure (see Fig. C.1). This method yields electron gases of very high mobility — exceeding $10^7 cm^2/Vs$ and a mean free path of many microns. These are amongst the most perfect conductors known.

In our discussion of semiclassics, we discussed the measurement of the Hall effect, and its classical analysis. Remember that in a magnetic field, a voltage develops perpendicular to the direction of current flow — the Hall voltage V_H — which must counterbalance the Lorenz force on the moving charges. The magnitude of this voltage is expected to be proportional to the current flowing between longitudinal contacts, and also linearly proportional to the magnetic field.

In general, we relate the current density to the electric field by

$$E_{\alpha} = \rho_{\alpha\beta} j_{\beta} \tag{C.1}$$



Figure C.1: Diagram of modulation-doped heterostucture [R.L.Willett, PhD Thesis, MIT 1988)]

or the inverse

$$j_{\alpha} = \sigma_{\alpha\beta} E_{\beta} \tag{C.2}$$

In an isotropic two dimensional system, we shall have $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{xy} = -\sigma_{yx}$. Note that σ and ρ are inverse matrices, so that

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} \tag{C.3}$$

$$\rho_{xy} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \tag{C.4}$$

Classically, the Hall resistance is

$$\rho_{xy} = R_H B = -\frac{B}{ne} \tag{C.5}$$

As noted above, it is linear in field.

Integer and fractional quantized Hall conductance

At high temperature, and low magnetic fields, linearity of the Hall resistance with magnetic field is always seen. But in high mobility samples, at low temperatures, and in large magnetic fields, a remarkable phenomena was discovered, as shown in Fig. C.2. The Hall resistance develops plateaux at rational fractions of the quantum of resistance

$$\rho_{xy} = \frac{h}{e^2} \frac{q}{p} \tag{C.6}$$

where q and p are integers. The case where q = 1 is called the integer quantum Hall effect (IQHE) and was discovered first. The general rational fraction is called the fractional quantum Hall effect (FQHE) and was discovered a little later, in samples with higher mobility. Corresponding to the plateaux in ρ_{xy} there are deep minima in ρ_{xx} . Note that the minima in ρ_{xx} correspond also to minima in σ_{xx} since when $\rho_{xy} \gg \rho_{xx}$, we have

$$\rho_{xy} \to 1/\sigma_{xy}$$
(C.7)

and

$$\rho_{xx} \to \sigma_{xx} / \sigma_{xy}^2 \quad . \tag{C.8}$$

As far as one can tell, the quantisation is exact — good to at least 1 part in 10^7 — and is now a laboratory resistance standard.

C.2 Landau level quantization

The orbital dynamics of an electron in two dimensions in a perpendicular magnetic field, in the absence of interactions and assuming a uniform potential are



Figure C.2: Transport data for the Hall effect of a 2D electron gas as a function of magnetic field. The top curve shows the integer Hall effect, and the lower curve, in a higher mobility sample, the fractional quantum Hall effect. The Hall resistance shows plateaux at $\rho_{xy} = (h/e^2) \times (1/i)$ for the integer QHE, and $\rho_{xy} = (h/e^2) \times (q/p)$ for the FQHE. A fully developed plateau in ρ_{xy} is accompanied by a deep minimum in ρ_{xx} [D.C.Tsui, Physica B **164** 59 (1990)]

described by the Hamiltonian

$$H = \frac{\hbar^2}{2m} (-i\nabla - \frac{e}{\hbar}\mathbf{A})^2 \tag{C.9}$$

where **A** is the vector potential so that the magnetic field is $\mathbf{B} = \nabla \wedge \mathbf{A}$.

The wavefunctions will depend on the gauge, and here we take the Landau gauge

$$A_x = -By \quad , \ A_y = 0 \tag{C.10}$$

so the Schr *o*dinger equation is

$$\frac{\hbar^2}{2m} \left(\left[-i\frac{\partial}{\partial x} - \frac{eB}{\hbar}y \right]^2 - \frac{\partial^2}{\partial y^2} \right) \psi = E\psi \tag{C.11}$$

Separating variables, we can take $\psi = e^{ikx}\phi(y)$, yielding

$$\frac{\hbar\omega_c}{2}\left(-l^2\frac{\partial^2}{\partial y^2} + \left[\frac{y}{l} - kl\right]^2\right)\phi = E\phi \tag{C.12}$$

which defines for us an energy scale (cyclotron frequency)

$$\hbar\omega_c = \frac{\hbar eB}{m} \tag{C.13}$$

and a length scale (magnetic length)

$$l^2 = \frac{\hbar}{eB} \tag{C.14}$$

The schrodinger equation describes a displaced harmonic oscillator, where the y-origin (kl^2) is proportional to the x-momentum k. The energy of the levels is independent of k, the usual ladder of eigenvalues

$$E_{nk} = \hbar\omega_c (n + \frac{1}{2}) \tag{C.15}$$

and corresponding wave-functions

$$\phi_{nk}(y) \propto H_n(y/l - kl) \times \exp\left[-(y - kl^2)^2/2l^2\right]$$
 (C.16)

where H_n is a Hermite polynomial.

There is a large degeneracy in each Landau level, which is determined by counting states. If we take L to be the length of the sample in the x-direction, and W the width in the y-direction, then $k = 2\pi s/L$, with s an integer. But since the centre of the level must lie in the sample $0 < kl^2 < W$, the total number of states in the Landau level is

$$N = \frac{LW}{2\pi l^2} \tag{C.17}$$

or more conveniently, that the number of states per unit area of a full Landau level is

$$n_B = \frac{1}{2\pi l^2} = \frac{eB}{h} = B/\phi_0 \tag{C.18}$$

where ϕ_0 is the flux quantum.

It is then convenient to measure electron densities in units of n_B , and we define the Landau level filling

$$\nu = n/n_B \tag{C.19}$$

Notice that we chose states that are extended in the x-direction, despite that there is nothing in the problem to single out the x-direction over the y. Since there is a massive degeneracy of states, we can in fact choose linear combinations of these states to produce eigenstates localised along y (or any other direction, for that matter.) It turns out *not* to be possible to produced eigenstates that are delocalised in all directions, and this is important.

Angular momentum eigenstates. The particular eigenstates above came out most easily because of our choice of gauge.¹ It is sometimes convenient to work with complex coordinates in 2D: z = x + iy; $\bar{z} = x - iy$; $\partial = \partial/\partial_x - i\partial/\partial_y$; $\bar{\partial} = \partial/\partial_x + i\partial/\partial_y$. In the symmetric gauge, $A = \frac{1}{2}B(1, -1)$, then the Hamiltonian becomes

$$H = \frac{\hbar^2}{m} \left[-2(\partial - \frac{\bar{z}}{4l^2})(\bar{\partial} - \frac{z}{4l^2}) + \frac{1}{2l^2} \right] \quad , \tag{C.20}$$

We can now work with eigenstates of both $L_z = \hbar (z\partial - \bar{z}\bar{\partial})$ and H,

$$\psi_{nm}(z\bar{z}) \propto \left(\frac{z}{\sqrt{2}l}\right)^m L_n^m(\frac{z\bar{z}}{2l^2})e^{-z\bar{z}/4l^2} \tag{C.21}$$

Here the L_n^m are Laguerre polynomials, n = 0, 1, 2, ... labels the Landau level, and m = -n, -n + 1, ... is the eigenvalue of the angular momentum. We shall later focus on the lowest Landau level, n = 0, when the Laguerre polynomial is a constant. In that case, the eigenstates all have the form

$$\psi_{0m} \propto (x+iy)^m e^{-(x^2+y^2)/4l^2}$$
 (C.22)

The eigenstates have a probability density that lies on a ring of radius $r_m \approx \sqrt{2ml}$, with a width of order l. Whereas the x-directed states are "tubes" strung along a line, these are rings.

Lastly, it should be evident from Eq. (C.22) that any wavefunction with the property that it lies in the lowest Landau level has the character $f(z)e^{-z\bar{z}/4l^2}$, where f(z) is an holomorphic or entire analytic function of z.

Spin. We shall suppress the discussion of spin, which at this level is subsumed by adding in the Zeeman energy of the electron $\pm 1/2g\mu_B B$, for the up

¹Remember of course that if we make a gauge transformation $A = A + \nabla \chi$, where χ is an arbitrary scalar field, then the wavefunction transforms to $\psi \to \psi e^{ie\chi\hbar}$.



Figure C.3: Density of states of a 2D uniform electron gas in a magnetic field. The flat density of states in zero field (light gray) is confined to sharp Landau levels at equal spacing $\hbar\omega_c$. The levels here are shown broadened, as produced by weak disorder — in a perfectly clean sample the states are δ -functions. The number of states in each level accounts for the area between the dashed lines at zero magnetic field.

and down polarised spin-half electron states. Each Landau level then splits into two. In GaAs, it turns out that the Zeeman splitting is about 60 times smaller than the cylcotron energy.

Disorder. Once we add any space dependent potential to the Hamiltonian, the infinite degeneracy of each Landau level will be broken, and the density of states will be broadened, as suggested by Fig. C.3. Almost all of the eigenstates are localised, though it turns out that there must be at least one that can carry a current from one side of the sample to another. One useful limit to visualise the states is in a smooth random potential, varying only on length scales much bigger than l.

If the potential is smooth, it is natural to expect that the wavefunctions corresponding to eigenstates in the tails of the density of states are localised either near the bottom of valleys, or the tops of hills, depending on whether the state is well below or well above the middle of the band. Remember that classically the orbits of an electron in a magnetic field move round equipotentials, one can expect that in this limit the eigenstates are tubes of width l that follow the equipotential contours. The orbital quantisation will be given by the Bohr-Somerfeld rule, that the phase accumulated around the orbit be a multiple of 2π . (Note that the wavefunctions of Eq. (C.22) are proportional to $r^m e^{im\phi}$, and approximately enclose an "area" $2\pi m l^2$, which contains m quanta of magnetic flux.)

In two dimensions, equipotentials are like contours on a map. Those at low energies, circulate round valleys, and at high energies, around hills. These are all localised wavefunctions — only a single contour constitutes and extended state. Note that in a magnetic field, the electron orbits in the opposite sense around a hill to a valley, and this topological change occurs at the percolation threshold.

C.3 Integer QHE

We are now in a position to go back and look at the transport data. It turns out that the IQHE can be largely understood in a picture where interactions are neglected.

Note that the number of states in each Landau level is proportional to the magnetic field. In Fig. C.4, we sketch how the chemical potential must adjust in the ideal system as the magnetic field increases. There are abrupt fields where the chemical potential drops from one Landau level into the next. These critical fields correspond to integer filling. These values of magnetic field line up nicely with the centres of the plateaux in the upper panel of Fig. C.2.

Now focus on the resistivity ρ_{xx} or equivalently σ_{xx} . The regimes of field where σ_{xx} is appreciable must be precisely when the chemical potential is passing through the middle of the Landau level and through the extended states. When



Figure C.4: The energies of the Landau levels spread out as a fan with increasing magnetic field. The chemical potential (thick solid line) adjusts to keep the total number of occupied states conserved, and repeatedly jumps between levels - at fields corresponding to integer filling $\nu = n2\pi l^2$, i.e. $B \propto 1/\text{integer}$.

the fermi level is within the regime of localised states, the diagonal conductivity is zero, and the Hall conductance cannot change — it must lie on a plateau. Note that both ρ_{xx} and σ_{xx} vanish together.

What about the *exact* quantisation? It can be constructed from a gauge argument. To simplify the story, we shall turn our sample into a *Corbino ring* (see Fig. C.5, where we assume that there is a current flowing around the ring, and therefore a Hall voltage V_H between the inner and outer edges. Now we imagine that we adiabatically thread a flux Φ into the central hole, so that eventually a whole flux quantum Φ_0 has been introduced. Note that states that do not extend around the hole cannot tell about the flux, but those that do pick up an Aharonov-Bohm phase

$$\int_C \mathbf{A} \cdot d\mathbf{r} = 2\pi \Phi / \Phi_0 \tag{C.23}$$

Now when the flux introduced is an integral number of flux quanta, the Hamiltonian, and hence the spectrum, is the same as before — the only thing that may change is the *occupancy* of the states. For the angular momentum states above, the process boosts the angular momentum quantum number from m to m+1. All the particles move out, and effectively one electron is shifted overall from the inside to the outside. In this case the work done is $\Delta U = eV_H$. If p electrons were to move (one from each occupied Landau level) the work is ptimes as large.



Figure C.5: Corbino disk geometry.

Separately, one may show quite generally (see your favourite QM text) that the induced current around the disk is related to the work done by

$$I = \frac{\partial U}{\partial \Phi} = \frac{\Delta U}{\Phi_0} = p \frac{e^2}{h} V_H \tag{C.24}$$

The point is that the *only* possible effect of the flux introduction is that an integer number of electrons are shifted from the inside to the outside of the ring — and that integer determines the Hall conductance.

C.4 Fractional QHE

This argument does not seem to allow for fractional quantisation. Suppose, however, that the system had a more complex set of eigenstates, and that in fact q flux quanta had to be introduced in order to return the system to itself. Then the argument would comfortably yield $\sigma_{xy} = \frac{p}{q} \frac{e^2}{h}$.

Such a result would also be straightforward if the excitations had not charge e, but charge e/q — and this is essentially the correct result. Such a state occurs because of the repulsive Coulomb interactions between electrons.

We will intuit our way to this result following the path trodden by Laughlin. We assume that we are at fields in the lowest Landau level, so that we will restrict ourselves to use single particle states of the form Eq. (C.22). We need to construct many-body wavefunctions where the particles keep away from each other, and also to satisfy antisymmetry.

The simplest antisymmetric state is a Slater determinant. The problem here is to choose which single particle states enter the Slater determinant – earlier we chose a set of single particle states that had the lowest kinetic energy, i.e. $|k| < k_f$. But the angular momentum eigenstates all have the same energy.

The only case that is simple is if we occupy all the states. Then the determinantal wavefunction will be

$$\psi_1 = \prod_{i(C.25)$$

This state has a density that corresponds to a filled Landau level, and is homogeneous in space.² Notice that antisymmetry is satisfied by having a node in the wavefunction sited on every particle. The state is unique — no other state can be constructed of the maximum density $\nu = 1$ while keeping to the lowest Landau level basis.

Now consider the states

$$\psi_{1/m} = \prod_{i < j} (z_i - z_j)^m \times \exp\left[-\sum_{k=1}^N z_k \bar{z}_k / 4l^2\right]$$
(C.26)

which are clearly special in the same way the filled Landau level is special. In order to satisfy antisymmetry, m must be an odd integer. This state should be of low energy because the nodes are "deep". And a little manipulation shows that this state has a density $\nu = 1/m$. (This can be seen approximately by noting that the maximum angular momentum for a single particle state is mN, corresponding to a radius $\sqrt{2mNl}$.) These "Laughlin fractions", $\nu = 1/3, 1/5, ...$ correspond to the most visible plateaux in experiment. Notice that even denominators do not appear in experiment.

Of course to understand transport in a many-body system, one needs not the ground state but the excitation spectra. Laughlin guessed an approximate wavefunction for a quasi-hole at position Z_0 , by the argument of threading through a flux quantum at that point - whereby each single particle state gets an angular momentum boost by 1, viz.

$$\psi_{hole} = \prod (z_i - Z_0) \psi_{1/m} \tag{C.27}$$

Note that since each single particle state has an occupation probability of 1/m, only a fraction 1/m of an electron is transported away from the hole — the charge is in effect e/m! One can solidify this result and take it further, to show that in fact these quasiparticles obey fractional statistics.

²Some trickery to convert the determinant where the columns are $1, z, z^2, z^3, \dots$ to the product is also needed.

This is only a taster of a very rich subject. One very productive way to view the FQHE states is the binding of multiple zeros of the wavefunction to individual particles, and it is this topological construct (rather than the accuracy of any particular form of the wavefunction — Eq. (C.26) is not exact) that enforces the exact statistics of the quasiparticles. The many higher states can be built up by hierarchical approaches, simply the 1/3 is the most robust.

Further reading

The Quantum Hall Effect, ed. R.E.Prange and S.M. Girvin, 2nd edition, Springer, 1990.

Appendix D

Magnetism

Magnetism is a phenomenon produced by interactions between electrons. Although the interactions in the Hamiltonian are *independent* of the electron spin, the effects of Pauli exclusion are such that the total energy depends on the spin configuration. Magnetic phenomena include not just the familiar ferromagnetism, but also *anti-ferromagnets* with more complicated magnetic order where the spins are ordered but not parallel, so there is no net magnetic moment. There are complementary views of magnetism as originating either from the alignment of *local moments* or from a spontaneous spin polarisation of itinerant electrons. We begin with the former.

D.1 Spin paramagnetism in metals

We first review the theory of Pauli paramagnetism. We consider a fermi gas with energy dispersion $\epsilon_{\mathbf{k}}$ in a magnetic field H. Because of the energy of the spin in a magnetic field, the spin-up and spin-down bands will be split (see Fig. D.1), and have energies

$$\begin{aligned} \epsilon_{\mathbf{k}\uparrow} &= \epsilon_{\mathbf{k}} + \mu_B H \quad , \\ \epsilon_{\mathbf{k}\downarrow} &= \epsilon_{\mathbf{k}} - \mu_B H \quad . \end{aligned} \tag{D.1}$$

Since the chemical potential must be the same for both spins, there must be a transfer of carriers from the minority spin band to the majority

$$n_{\uparrow} - n_{\downarrow} = \mu_B H g(\mu) \tag{D.2}$$



Figure D.1: Spin-split bands in the Stoner approximation

where $g(\mu)$ is the density of states at the Fermi level¹. The magnetisation is $M = \mu_B(n_{\uparrow} - n_{\downarrow})$ which then gives us the static spin susceptibility

$$\frac{M}{H} = \chi_{\sigma} = \mu_B^2 g(\mu) \quad . \tag{D.3}$$

D.2 Ferromagnetism in the Stoner-Hubbard model

Now let us include in a very simple fashion the effect of interactions. Remember how in the Hartree-Fock theory of the electron gas we found that the effect of exchange was to lower the energy of the fully spin-polarised state with respect to the paramagnet. (See A.4). In the Stoner-Hubbard model we postulate an effective interaction U between up and down spin densities

$$\dot{H}_{int} = U n_{\uparrow} n_{\downarrow} \quad , \tag{D.4}$$

The energies of the two spin bands are now (see Fig. D.1)

$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}} + Un_{\downarrow} + \mu_B H$$

$$\epsilon_{\mathbf{k}\downarrow} = \epsilon_{\mathbf{k}} + Un_{\uparrow} - \mu_B H$$
(D.5)

With the same approximation as before - that the density of states can be taken to be a constant, we can then self-consistently determine the average spin density

$$n_{\uparrow} - n_{\downarrow} = [U(n_{\uparrow} - n_{\downarrow}) + 2\mu_B H] \frac{1}{2} g(\mu) \quad . \tag{D.6}$$

¹Obviously, we must assume that the splitting is small enough that the density of states can be taken to be a constant. We define $g(\mu)$ to be the density of states for both spins.

The magnetisation is $M = \mu_B(n_{\uparrow} - n_{\downarrow})$ which then gives us the static spin susceptibility

$$\chi_{\sigma} = \frac{\mu_B^2 g(\mu)}{1 - \frac{Ug(\mu)}{2}} \quad . \tag{D.7}$$

In comparison to the non-interacting case, the magnetic susceptibility is enhanced, and will diverge if U is large enough that the Stoner criterion is satisfied

$$\frac{Ug(\mu)}{2} > 1$$
 , (D.8)

which marks the onset of ferromagnetism in this model.

D.3 The origin of local magnetic moments

Strongly-bound core states in atoms acquire magnetic moments because of interactions between electrons. The general rule is that many-particle wavefunctions that are built out of *orthogonal* orbitals have a tendency to spin-alignment. This is one of the Hund's rules, and can be understood easily within the Hartree Fock approximation.

As a simple example, consider a model atom with two orbitals of singleparticle energies $E_{A,B}$ in which we wish to accommodate two electrons (Fig. D.2). Often they will be of similar, or identical energies, but for definiteness, let's take $E_A < E_B$. Within Hartree-Fock (see Eq. (A.15)) in this simple model,



Figure D.2: Possible low energy configurations of two electrons in a two-level atom

there are the following interaction terms: the direct (Hartree) terms

$$Q_{AA} = \langle AA | \frac{e^2}{r_{12}} | AA \rangle$$

$$Q_{AB} = \langle AB | \frac{e^2}{r_{12}} | AB \rangle$$

$$Q_{BB} = \langle BB | \frac{e^2}{r_{12}} | BB \rangle$$
(D.9)

and the exchange energy

$$J_{AB} = \langle AB | \frac{e^2}{r_{12}} | BA \rangle \tag{D.10}$$

that operates only betgween configurations where the single particle states are occupied with identical spin. Since the orbitals are assumed orthogonal, then $Q_{AA} \approx Q_{BB} \gg Q_{AB} \approx J_{AB}$

The three configurations have the energy shown in Fig. D.2; two are singlets, and the last is a triplet. The triplet configuration will have the lowest energy if

$$Q_{AA} - Q_{AB} + J_{AB} > E_B - E_A \tag{D.11}$$

which is very commonly the case when Q_{AA} is large.

This simple example reflects a general phenomenon, seen clearly with wavefunctions that can be factorised into a product of orbital and spin components. Because the total wavefunction must be antisymmetric, if we choose the spin wavefunction to be symmetric under exchange of coordinates (which here enforces a triplet: one of $|\uparrow\uparrow\rangle; |\downarrow\downarrow\rangle; 2^{-1/2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$)then the spatial part of the wavefunction is *anti*- symmetric. The singlet state $2^{-1/2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is antisymmetric in spin space, and therefore the real space wavefunction must be symmetric. An antisymmetric wavefunction must have nodes whenever two spatial coordinates are equal: $\psi(\dots, r_i = r, \dots, r_j = r, \dots) = 0$. So it is then clear that the particles stay farther apart in an antisymmetrised state than in a symmetric state, and because of the Pauli principle an antisymmetric wavefunction (which will generally have high spin) has lower energy.

The physical reason for the existence of local moments on atoms is then a combination of the Pauli principle together with repulsive interactions between ions. If we consider, say, d-levels in an ion, since the d-states are degenerate, we shall always get high spin configurations. However, in the environment of a solid, the d-levels are split because the atom is no longer in a potential of spherical symmetry. If this *crystal field splitting* is large enough, then the condition of Eq. (D.11) will not be satisfied, and the orbitals will be filled one after another - and generally the atom will have low spin.

D.4 Types of magnetic interactions

The existence of magnetic moments locally on atoms is only part of the story of magnetism, because to obtain an ordered magnetic ground state, the moments between neighbouring atoms must be coupled. There are a number of different ways that these couplings can arise. The net effect of the couplings between neighbours can in the end usually be parametrised quite simply, just in terms of pairwise interactions between spins *on neighbouring sites*, viz.

$$H_{spin} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{D.12}$$

44

This is the Heisenberg model, which now couples the total spin on an atom (which will be determined by the solution of the atomic problem) to that of its neighbours. Notice that the coupling only depends on the relative orientation of the spins, and not on their absolute direction relative to the crystal lattice. When the angular momentum of the ion contains an orbital part as well as a spin part, then the spin Hamiltonian will include a piece that depends on the *absolute* spin direction.

Dipolar Interaction

The first idea might just be that the moments could couple via through the magnetic fields they generate. However, this is very small: the energy of interaction of two magnetic dipoles of strength m at a distance r is of order $\mu_o m^2/4\pi r^3$. Putting in a magnetic moment of order a Bohr magneton, we get

$$U_{dipolar} \approx \frac{\mu_o}{4\pi} (\frac{e\hbar}{2m})^2 \frac{1}{r^3} \approx \pi \alpha^2 (\frac{a_{Bohr}}{r})^3 Ryd.$$
(D.13)

where $\alpha \approx 1/137$ is the fine structure constant. At typical atomic separations of 2nm, this is about 4×10^{-5} eV, or less than a degree Kelvin. As always, magnetic interactions are over-ruled by charge interactions, and such energy scales are rarely important.²

Dipolar terms do play an important role in the domain structure of magnets, once the spins have already been aligned by other means.

Direct exchange

The intra-atomic exchange interaction we discussed in Sec. D.3 is an example of *direct exchange*, because it comes from interactions between *overlapping* orbitals. When the orbitals concerned are orthogonal, J is *positive* in sign, i.e. the lowest energy state is a triplet. However, if the overlapping orbitals are not orthogonal – as will happen between two orbitals between neighbouring atoms – the interaction may be of a *negative* sign, so the lowest energy is a singlet.

Qu.4.3 Covalent bonds are singlets How is it that electrons in a covalent bond - e.g. H_2 - are almost invariably in singlet states? The two atomic states that make up the wavefunction are not orthogonal, and so the charge density is not independent of the spin-state of the ions. The singlet state will lead to a charge density that is more favourable for strong bonds than the triplet.

Consider single-particle wavefunctions on two neighbouring identical atoms ψ_A , ψ_B , which may be assumed real. These are to be used

²Interactions between electrical dipoles – as occurs in a ferroelectric – are not negligible. Here we get the same expression but without the factor of α^2

as the basis for a two-electron state. Show that the charge density in a singlet (triplet) state made out of the two orbitals is given by

$$\rho(r) = |\psi_A(r)|^2 + |\psi_B(r)|^2 \pm 2 < \psi_A |\psi_B > \psi_A(r)\psi_B(r) \quad . \tag{D.14}$$

By reference to Fig. D.3, explain why the singlet state will usually be lower in energy.



Figure D.3: A sketch of the charge density for the wavefunctions in a singlet state (solid line) and a triplet state(dotted line) for two overlapping gaussian orbitals in Eq. (D.14)

Indirect exchange in metals

In a d- or f-band metal, such as Fe, there are both localised electrons with a moment derived from the tightly bound orbitals, and *itinerant* electrons derived from the s-p bands. The itinerant bands are weakly, if at all, spin-polarised by themselves because the exchange interactions are small and the kinetic energy large. However, the itinerant carrier acquires an *induced* spin polarisation due to its interaction with the core spin on one atom. This spin polarisation can then be transmitted to a neigbouring ion, where it attempts to align the neighbouring spin. There is then an interaction, often ferromagnetic in character, produced by this mediated interaction, often called RKKY (for Ruderman-Kittel-Kasuya-Yoshida).

A more detailed view of this process can be given. If we have an ion of spin ${\bf S}$ embedded in the conduction electrons, one would expect that the local direct exchange



Figure D.4: . In metals, a local moment will polarise the conduction electron spins, producing a spin density that decays away and oscillates in sign with period $1/2k_F$. The interaction of the induced spin density with a neighbouring local moment produces the RKKY interaction

will give rise to a contact interaction of the form

$$H_{int} = -J\mathbf{S} \cdot \mathbf{s}\delta(\mathbf{r}) \quad , \tag{D.15}$$

with s the conduction electron spin density, and J a direct exchange interaction. The spin density is not otherwise polarised, but the perturbation will induce a weak spin density modulation in the conduction cloud, which will of course decay away to zero at large distance from the ion. The induced spin density is just

$$s(\mathbf{r}) = J\chi_{\sigma}(\mathbf{r})S\tag{D.16}$$

where we have introduced the spin susceptibility χ_{σ} . (Above we considered the average spin susceptibility to a uniform field, this is a generalisation to non-uniform fields).

At a nearby lattice site (say \mathbf{R}), the induced spin density caused by the polarisation of one atom interacts with the spin of another, and the energy is then

$$-J\mathbf{S}(\mathbf{R}) \cdot \mathbf{s}(\mathbf{R}) = J^2 \chi_{\sigma}(\mathbf{R}) \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(0) \quad , \tag{D.17}$$

Summing over all pairs of sites in the crystal we obtain

$$H_{RKKY} = -\sum_{ij} J^2 \chi_{\sigma}(\mathbf{R}_{ij}) \mathbf{S}(\mathbf{R}_i) \cdot \mathbf{S}(\mathbf{R}_j) \quad . \tag{D.18}$$

If we could replace $\chi_{\sigma}(\mathbf{R}_{ij})$ by its average (say Eq. (D.3)) then one would predict a long range ferromagnetic interaction, which is not far from the truth for many materials. Of course, in a more accurate theory, χ decays as a function of distance. A careful analysis shows in fact that χ oscillates, changing sign as it decays, with a wavelength π/k_F . The origin of these *Friedel oscillations* is the fermi sea itself. Since the electron gas occupies states of momenta smaller than k_F , it is not possible for it to respond to a spatial frequency faster than $2k_F$, and there is a sharp kink in $\tilde{\chi}(q)^3$ at the momentum $q = 2k_F$. Sharp features in momentum space give rise to oscillations in real space for the fourier-transformed $\chi(r)$, appearing as oscillations visualised in Fig. D.4.

We saw that χ_o is of order $g(\mu)$, the density of states per unit energy, so the the Heisenberg interatomic exchange parameter is of order $J^2N(\mu)$ which can be large - up to fractions of an eV.

Superexchange and insulating antiferromagnets

When there is strong overlap between the orbitals as in a typical covalent bond, the energy lowering of the singlet state is subtantial, and the system has no

³Here $\tilde{\chi}(q) = \int dr \exp(iq \cdot r)\chi(r)$ is defined in fourier space

magnetic character. However, a special class of much weaker interactions can be important when two magnetic moments are separated by a non-magnetic ion (often O^{2-}) in an insulator. There is a small overlap of the magnetic orbitals occurring on the mediating non-magnetic ion, and the system lowers its energy by having some increased density on the this ion. Just as in H_2 , this overlap is favoured in a singlet state.

In this insulating situation, the electronic structure is ionic, not covalent, so it is not possible to form a complete singlet ground state (crudely, each atom will have several neighbours, and cannot choose a single neighbour to pair with). An alternative state has the spins anti-aligned,

$$|\uparrow\downarrow\rangle$$
 (D.19)

rather than in a total singlet,

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{D.20}$$

When extended throughout the solid, Eq. (D.19) describes an *antiferro-magnet*, where alternate sites have antiparallel spins (see Fig. D.5). On more complicated lattices, very complex arrangements of spins can result.

The magnitude of this interaction is often quite small, in the range of a few to a few hundred degrees Kelvin. Consequently, these systems will often exhibit phase transitions from a magnetically ordered to a disordered paramagnetic state at room temperature or below.

D.5 Collective magnetic properties

D.5.1 Magnetic phase transitions

The Heisenberg model, however complicated the mechanisms that generate the interactions, provides a very good description of the low energy spin dynamics of many magnetic materials.

For most purposes, and especially to describe phenomena at finite temperatures, it turns out that the spins can be treated classically and so the analysis of magnetic ground states and magnetic ordering becomes a topic in classical statistical physics, that is somewhat removed from the agenda of this course. Because the interaction J is usually small in comparison to other electronic energies in the problem, we need to include the thermal fluctuations only of the spins at low temperatures, because other degrees of freedom are comparatively stiff, so produce only small changes to the free energy at the temperatures where macroscopic magnetic phenomena are seen. The transition temperature of a magnet is determined by a competition between the energetics of the interaction between spins – favouring ordering – and the entropy, which is larger in a disordered state. Only in rare cases do we need to go beyond simple classical



Figure D.5: . Schematic picture of the ground state of a ferromagnet and an antiferromagnet. The order parameter for the ferromagnet is the uniform magnetisation, and for an antiferromagnet it is the $\langle \mathbf{S}(\mathbf{Q}) \rangle$, where \mathbf{Q} is the wavevector corresponding to the period of the order

models of interacting moments to understand the magnetic behaviour of real materials.

Depending on the sign of J, the ground state will be ferromagnetic (aligned spins) or anti-ferromagnetic (anti-aligned spins on neighbouring sites); more complicated magnetic states can arise if we have different magnetic ions in the unit cell, and also on taking account of magnetic anisotropy.

While it is straightforward to measure the magnetisation in a ferromagnet, measuring the order parameter of an antiferromagnet is more tricky because it corresponds to spins ordering with a finite wavevector. Such order can, however, be cleanly observed by elastic neutron scattering (see Fig. D.8).

D.5.2 Spin waves

We learned earlier that a consequence of having a periodic lattice is that small amplitude dynamical modes exist - phonons, or sound waves. In a solid with magnetic order, the analogous modes are small oscillations of the spin magnitude and direction, known as spin waves.

In the magnetically ordered state, the picture is different, and we will consider here the case of a ferromagnet, starting from the nearest neighbour Heisenberg Hamiltonian

$$H_{Heis} = -J \sum_{i,j=n.n} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \tag{D.21}$$

The spin variables are angular momenta, and as such they satisfy the commutation relations for angular momenta

$$[\hat{S}_{\alpha}, \hat{S}_{\beta}] = i\hbar\epsilon_{\alpha\beta\gamma}\hat{S}_{\gamma} \quad , \tag{D.22}$$

where the subscripts in Eq. (D.22) refer to the cartesian axes (x, y, z), whereas those in Eq. (D.21) are the site labels.



Figure D.6: The top figure shows the classical picture of a spin wave generated by an array of precessing spins; the bottom figure shows the same viewed from the top.

We can use these two equations to obtain the Heisenberg equation of motion for a spin at a single site

$$\dot{\hat{\mathbf{S}}}_{n} = -\frac{i}{\hbar} [\hat{\mathbf{S}}_{n}, H_{Heis}] = \frac{2J}{\hbar} \sum_{j=n.n. \ of \ n} \hat{\mathbf{S}}_{n} \wedge \hat{\mathbf{S}}_{j}$$
(D.23)

To derive this, we need to assume (correctly) that spin operators on *different* sites commute. The factor of two in this equation comes about because H_{Heis} contains a sum over all pairs i, j, and the commutator will pick out terms with both i = n and j = n.

Notice that the form of this equation is that it describes precession of the spin at site *n* about the effective exchange field $J \sum_j \hat{\mathbf{S}}_j$ of the nearest neighbour spins. While this is a fully quantum mechanical problem, we can gain insight (and the correct answer when the magnitude of the spin is large) by treating this in a semiclassical approximation.⁴

We can assume that in the ordered state there is a uniform ferromagnetic moment $\langle \mathbf{S} \rangle = S\hat{z}$, which we have chosen to point in the z-direction. We shall now look for the collective modes of small amplitude spin fluctuations about the magnetically ordered ground state. One can guess the form of the solutions by considering a single spin tilted from its axis by a small angle, while the neighbouring spins are held fixed - in this case the spin will simply precess in a circle about the \hat{z} -axis. But of course the motion of one spin will affect the others, so the precession of a single spin will not be an eigenstate; but if all of the spins precess in such a way as to keep the relative angles between neighbours constant, then we can have a wave with uniform precessional rate. This is shown pictorially for a one-dimensional chain in Fig. D.6

To get the dispersion relation for the spin wave mode, we write

$$\hat{\mathbf{S}}_n = S\hat{z} + \delta \mathbf{S}_n \tag{D.24}$$

 $^{^{4}}$ The quantum mechanical case is not much more difficult, but involves making a different representation for the quantisation of the spins; see Marder pp 753-757.



Figure D.7:

where $\delta \mathbf{S}_n$ is a vector lying in the x - y plane. Substituting this into Eq. (D.23) we get

$$\delta \dot{\mathbf{S}}_n = \frac{2JS}{\hbar} \sum_{j=n.n. of n} (\delta \mathbf{S}_n - \delta \mathbf{S}_j) \wedge \hat{z}$$
(D.25)

The equation in now classical – all the operators have been approximated by classical vectors.

By considering two neighbours of the n^{th} spin, as in Fig. D.7, each at relative angles θ , one can show that the rate of precession according to Eq. (D.25) is

$$\omega = \frac{4JS}{\hbar} (1 - \cos\theta) \quad . \tag{D.26}$$

Thus for a spin wave of wavevector q, the dispersion is

$$\hbar\omega = 4JS(1 - \cos(qa)) \quad . \tag{D.27}$$

The generalisation to a three-dimensional lattice is quite straightforward:

$$\hbar\omega_{SW}(\mathbf{q}) = 2ZSJ(1 - \frac{1}{Z}\sum_{\mathbf{R}=n.n.} e^{i\mathbf{q}\cdot\mathbf{R}}) \quad , \tag{D.28}$$

where Z is the number of nearest neighbours. Notice that as $\mathbf{q} \to 0$, $\omega \propto q^2$.

We are of course not surprised to find the mode frequency vanishing in the long-wavelength limit, because at q = 0, this mode would be a uniform tilting of all the spins in the whole lattice. The Heisenberg model knows only about relative directions of spins, so this must have zero energy; our choice of the z-direction for the ordered moment was completely arbitrary. However, the quadratic - rather than linear, as for phonons - behaviour is a consequence of a further conservation law – the total spin $\sum_i \hat{\mathbf{S}}_i$ commutes with the Hamiltonian Eq. (D.21). In the case of the Ferromagnet this means the order parameter is conserved and the quadratic dependence is a characteristic of ferromagnetic spin waves; spin waves exist also in antiferromagnetically ordered states, but their momentum dependence is indeed linear in that case.

D.5.3 Neutron scattering

Neutron scattering is an ideal probe for the observation of typical magnetic fluctuations in solids, because the characteristic energy and momentum range of spin fluctuations is comparable to the energy-momentum dispersion of neutrons available either from reactor or "spallation" sources. Neutrons have a magnetic moment, and therefore interact with magnetic electronic fluctuations, as well as directly with the nucleus.

Reactor sources of neutrons operate continuously, and the energy range of the neutrons is determined by thermalising with a surrounding moderator. This produces beams with a broad band of wavelengths. In a spallation source, neutrons are produced by the bombardment of a heavy metal target with energetic particles from an accelerator. Specific wavelengths can be separated out by scattering from a single crystal monochromator – that operates in essentially the same way as a diffraction grating for light – or by a "chopper" spectrometer that selects the velocity directly.

The neutron-nucleus interaction makes neutron scattering a useful probe for crystal structure determination (elastic) and determining phonon dispersion relations (inelastic). The magnetic interaction allows neutrons to be used as a probe to determine the magnetic ordering of magnetic ground states (by elastic scattering), and to determine the magnetic fluctuation spectrum by inelastic scattering.

Its value is best displayed by showing some data. Fig. D.8 shows elastic magnetic scattering determining the existence of an antiferromagnetic ordered phase⁵. and Fig. D.9 shows how inelastic neutron scattering can be used to determine the dispersion relations of spin waves in a ferromagnet⁶.

⁵R.Plumier, data quoted by Kittel, p 698

⁶T.G. Perring *et al.*, Physical Review Letters **77**, 711 (1996)



Figure D.8: Elastic neutron scattering on MnV_2O_4 , which is an antiferromagnet with a transition temperature of $T_N = 56K$. The angular scan measures the angle of diffraction of the neutrons, and two magnetic peaks can be seen, that decrease in intensity as the temperature is raised.



Figure D.9: Inelastic neutron scattering from the ferromagnet $La_{0.7}Pb_{0.3}MnO_3$, which is well described as a Heisenberg ferromagnet, at 10K. The upper figure shows a slice of the spectrum at a constant energy transfer of approximately 7 meV, as a function of momentum near the (100) reciprocal lattice point. The two peaks correspond to excitation of spin waves of well-defined momentum, with the width of the peaks in the figure given entirely by the experimental resolution. The lower figure maps out the full dispersion relation of the spin waves in the major symmetry directions, using multiple scans of the type shown above (the material is a cubic perovskite, and the magnetic Mn ions lie on an f.c.c. lattice). The solid line is a fit of the dispersion curve to a nearest neighbour Heisenberg model, with an exchange constant 2JS = 9 meV; the dotted line corresponds to a slightly different theoretical model – whose distinction from the Heisenberg model is of no consequence to our discussions.

Appendix E

Heavy fermions

E.1 The electron as a collective excitation

The title of this section seems rather perverse, because we surely know that an electron is a fundamental particle. But in a solid, the an *individual* electron cannot be separated from the rest of the interacting quantum liquid, so the existence of individual particles is moot. Instead, we should think of the kind of experiments we might do to study "electron-like" excitations.

In a non-interacting system, the electrons go into band eigenstates. If we include the electron-electron interactions in an average fashion - e.g. Hartree or Hartree-Fock theory - then we still have the concept of bands (whose energy is changed by the interactions) that are discrete eigenstates with a single-particle like index. But this is clearly an approximation, and what can in fact survive beyond this?

In a real experiment, we do not measure the ground state properties but the excitations. One simple excitation is the addition or removal of an electron to the system: e.g. via tunnelling or photoemission. If we put a particle into a single-particle eigenstate of the Hamiltonian labelled by its momentum \mathbf{k} , then the wavefunction will evolve in time following the Schrödinger prescription

$$\psi_k(\mathbf{r},t) = \psi_k(\mathbf{r})e^{-i\epsilon_{\mathbf{k}}t} \quad . \tag{E.1}$$

Here ψ_k is the Bloch wavefunction satisfying the time-independent Schrödinger equation, and the time-dependent solution oscillates in time with a single frequency $\omega = \epsilon_{\mathbf{k}}$, the band energy.

What about an interacting system? If we add a particle, it will collide, interact, and exchange with all the other particles in the system, but supposing the interactions are weak (though they aren't) one might imagine that something similar to the particle will survive.

First, if we fix the momentum \mathbf{k} of the excitation, that cannot change be-

cause the two-particle interactions conserve momentum. Of course, some of the character of the original particle will now be shared with a "cloud" of electrons screening it.

Second, since we can see that in a metal there is a continuum of excitations, we should expect it to decay with a finite lifetime - say $1/\Gamma_{\mathbf{k}}$. The timedependence of the state will now become $e^{(i\epsilon_{\mathbf{k}}-\Gamma_k)t}$.

Third, there is no reason that the dispersion relation should be the same as for the free particle: we should replace $\epsilon_{\mathbf{k}}$ by a renormalised $\tilde{\epsilon_{\mathbf{k}}}$. This latter is often referres to as a mass renormalisation: $m^*/m = \epsilon_{\mathbf{k}}/\tilde{\epsilon_{\mathbf{k}}}$.

This propagating (and decaying) object we call a *quasi-particle*. If $\Gamma_{\mathbf{k}}$ is small, then the quasiparticles are long-lived and have some real meaning. They also have charge e and spin $\frac{1}{2}$; we will not mess with Fermi statistics here.

The Fermi liquid

Why is it that Γ can be small in a metal where the typical separation between electrons is only an Angstrom or so? The answer is provided by Fermi statistics, and is codified in Landau's theory of the Fermi liquid. In short, the fact that Fermi statistics exclude double occupancy of the same quasiparticle state *quarantees* that

$$\Gamma \propto (\omega - \mu)^2$$
 . (E.2)

So for excitations close to the fermi surface, the lifetime becomes very long. Furthermore the quasiparticle states are in one-to-one correspondence with the states of the non-interacting system - which means that the volume of the fermi surface is unchanged.

This is an extraordinarily important result for metals. It explains why it is that the mean free path in, e.g. copper, is very long at low temperatures if the material is pure enough, despite the fact that the characteristic separation between electrons is of order a lattice constant and their interaction energy is of order a few eV. The electrical current is carried by a quasiparticle excitation that is a collective mode of the fermi system. In the language of perturbation theory, the quasi-particle is a "dressed" excitation, that involves a correlated motion of the added electron together with the many-body background.

Here is a sketch of how to obtain that result. Let us assume that quasiparticles exist, and estimate the effect of the interactions between them. So in Fig. E.1 we show the Fermi sea, with a test particle (1) added – of course it has to be placed above the chemical potential because the states below are filled. Now consider the interaction of this particle with a particle (2) (which must be inside the Fermi sea). The result of the collision will be scattering to final states labelled (1', 2'). The final states must have initially been empty (Fermi statistics), so both 1' and 2' must lie at energies above the chemical potential μ . But we also have to satisfy energy (and momentum) conservation

$$\omega_1 + \omega_2 = \omega_{1'} + \omega_{2'} \quad , \tag{E.3}$$

which means that

$$\omega_1 + \omega_2 > 2\mu \quad . \tag{E.4}$$



Figure E.1: Collision between two quasiparticles near the Fermi surface. The initial and final states are marked by open and filled circles.

We can rewrite this as

$$\mu - \omega_2 < \omega_1 - \mu \quad . \tag{E.5}$$

We see that the only particles which are allowed to scatter from the test particle 1 are those whose energy is closer to the Fermi energy than particle 1 itself. So if $\omega_1 \to \mu$, there are no scattering processes allowed, and the quasiparticle is long-lived.

There is a further constraint according to momentum conservation. The momentum transfer in the scattering process takes particle 1 from state \mathbf{p} to $\mathbf{p} + \Delta \mathbf{p}$, with exactly the same momentum transfer in reverse for particle 2. We can separate the components of the momentum transfer perpendicular and parallel to the Fermi surface, and it is clear that $\Delta \mathbf{p}_{\perp} < v_F(\omega_1 - \mu)$, where v_F is the Fermi velocity. In order to calculate the overall scattering rate, we need to integrate over all the possible final states, and over all the possible states of particle 2. What is important in what follows is that two of these integrals are constrained: the energy of particle 2, and the momentum transfer perpendicular to the FS. We can now estimate that the scattering rate must be of order

$$\Gamma(\omega_{1}) \propto \int_{2\mu-\omega_{1}}^{\mu} d\omega_{2} \int_{0}^{v_{F}(\omega_{1}-\mu)} d\mathbf{\Delta}\mathbf{p}_{\perp} \int d(other \ momenta) W(1,2;1',2')$$

$$\propto W(\omega_{1}-\mu)^{2} \tag{E.6}$$

where W is the scattering matrix element, which we replace by its average value near the Fermi surface. So $\Gamma \to 0$ for quasiparticles whose energy lies exactly on the Fermi surface, and our assumption that quasiparticles exist and are long-lived is self-consistent. Moreover, it can be shown that the quasiparticles are in a one-to-one correspondence with the particles of the noninteracting theory.¹

This is an existence proof of the quasiparticle concept, but of course it does not guarantee that the Fermi liquid state always exists. It can be shown that turning on the interaction between particles adiabatically from zero then the free particles smoothly transform into quasiparticles, and the volume contained

¹The proof is formidable, and is known as Luttinger's theorem : J.M.Luttinger and J.C.Ward, *Physical Review* **118**, 1417 (1960); *ibid.* **119**, 1153 (1960). See also the book by A.A.Abrikosov, L.P.Gor'kov, and I.E.Dyalozhinski, *Methods of Quantum Field Theory in Statistical Physics*, Dover Edition, 1975

within the Fermi surface is unchanged (this is the Luttinger theorem). However, this does not preclude a phase transition, where the Fermi liquid character abruptly disappears. The conditions under which fermi liquids exist or not is an active field of both experimental and theoretical research.

d- and f-band metals

Fermi liquid theory is inexorable, and provided there is not a phase transition², the fermi surface of a non-interacting system evolves continuously and smoothly into the fermi surface of an interacting system. The volume of the fermi sea cannot change, because there are as many quasiparticles as real particles. This is true even in the case when the interactions become very large.

So an interesting place to look is at metals made up out of d- and especially f-electron bands. Particularly in the latter case, we have tightly bound orbitals that overlap very weakly with the neighbours, and we expect the bandwidth (which measures the average kinetic energy) to be very small. However, the Coulomb repulsion between two electrons on the same site is big.

In intermetallic compounds such at UPt_3 and $CeCu_6$, band structure calculations would tell us to expect that s, p, and d electrons from the transition metal as well as f electron wavefunctions from the actinide or rare earth contribute to states at the fermi surface. But one might expect that the f-orbitals are so localised that they are part of the atomic "core", so the band-theory result looks dubious. However, we shall see that their hybridisation with the more extended *s*-electron states derived from the transition metal leads in the end to their complete metallic character, as predicted by the fermi liquid theory.

E.2 Local moments and the Kondo effect

Before thinking about dense arrays of f-orbitals embedded in a metal, we consider the case of a single isolated local level in a metal. This seems straightforward, but produces a surprise.

We discussed earlier the idea of "local moments", that arise because the Coulomb repulsion on a site favours the alignment of spins of the local eigenstates. We now ask what happens when a local moment is put into a metal. Indeed, it is often that case that a magnetic impurity (say Fe) added into a normal metal (say Cu) keeps its magnetic moment. Let us assume that we are in the extreme correlated limit, so the charge in the localised state is fixed and the only remaining degree of freedom is a spin S. Here we consider $S = \frac{1}{2}$. The

 $^{^2{\}rm For}$ example, magnetism or a charge-density wave instability introduce new long-range order and therefore change the topology of the fermi surface

interaction term is then just exchange

$$H_{Kondo} = J \sum_{i} \mathbf{S} \cdot \sigma_i \tag{E.7}$$

where the sum is over all the electrons in the metal, which is adequately described by free electrons, with a density of states $g(\mu)$ at the chemical potential. Electrons in the fermi sea can then collide with the local moment, flipping its spin (and also losing momentum in the process) — consequently this scattering contributes to the resistivity of the metal. Perhaps puzzling however, is that if J is positive (*anti*-ferromagnetic coupling), the scattering grows as the temperature is lowered (so the resistivity increases), an effect first explained by Kondo (see Fig. E.2).



Figure E.2: . Kondo effect. The resistance of a metal with dilute magnetic impurities increases as temperature is lowered, with a theoretical form (solid line) $\rho = -\rho_o \log(T/T_K)$ [J. Kondo, 1964, Prog. Theor. Phys. **32**, 37]. Data from MacDonald et al (see Kittel)].

It turns out that below a temperature called the *Kondo* temperature

$$T_K = \frac{1}{k_B \bar{g}(\mu)} e^{-1/(\bar{g}(\mu)J)}$$
(E.8)

the strong scattering resolves itself as the local moment binds into a singlet state with electrons taken from the fermi sea³. The overall moment disappears as the local spin is "dressed" by a cloud from the fermi sea; at the same time

³Here we define $g(\mu) = \frac{N}{V}\bar{g}(\mu)$, so that \bar{g} has dimensions of (energy)⁻¹ and a value approximately equal to the inverse of the bandwidth.

the resistivity grows as the dynamical scattering of the electrons in the fermi sea with the local moment increases.

E.3 Experimental properties of heavy fermion systems

In f-band metals like UPt_3 , the f-electrons are not dilute, so even when the Kondo effect has been operative, the "dressed" singlets can hop between sites, forming an itinerant band. The band-width turns out to be extremely small, and the coherent metallic behaviour then appears only at low temperatures. We briefly discuss the experimental signatures of this crossover in heavy fermion systems.

Magnetic susceptibility

Moments lead to a magnetic response, and if there was a set of free spins, then we should see a Curie law.

$$\chi = \frac{\partial M}{\partial H} = \frac{N}{V} \frac{(g_L \mu_B)^2}{3} \frac{J(J+1)}{k_B T}$$
(E.9)

for a set of ions of angular momentum J, and g_L the Landé g-factor.

Qu.5.4 Curie Law An exercise in statistical physics that you may well have seen before.

Using

$$M = -\frac{1}{V}\frac{\partial F}{\partial H},\tag{E.10}$$

and the partition function

$$Z = e^{-\beta F} = \sum_{J_z = -J}^{J} e^{-\beta g_L \mu_B H J_z} \quad \beta = 1/k_B T , \qquad (E.11)$$

derive the Curie law Eq. (E.9), and the conditions for its validity.

Fig. E.3 shows the magnetic susceptibility of UBe_{13} which shows a large moment at high temperatures, but rather than continuing to follow a Curie law to low temperatures — or ordering magnetically — the susceptibility saturates at large values in a metallic state.



Figure E.3: . Inverse magnetic susceptibility of UBe_{13} showing a Curie law at high temperatures and a large local moment. At low temperatures, the susceptibility saturates to a constant, without the appearance of magnetic order.[Ott et al, in *Local Moment Formation in Solids*, ed W.J.L.Buyers, (Plenum NY) 1984, p 305.]

Electronic specific heat

A revealing view of this class of materials comes from the specific heat. The general form of specific heat that we should see in a metal at low enough temperature is

$$C = \gamma T + \alpha T^3 \tag{E.12}$$

where the first term is the electronic contribution and the second comes from the lattice The electronic contribution depends on the density of states $g_{eff}(\mu)$ at the fermi energy, viz.

$$\gamma = \frac{\pi^2}{3} k_B^2 g_{eff}(\mu) \tag{E.13}$$

For a conventional metal, one usually finds $\gamma \approx \text{few } mJ/moleK^2$, whereas here (Fig. E.4) the number is much larger. If these are truly electronic quasiparticles, they have a very large density of states at the fermi surface, or indeed a very heavy mass — hence the name *heavy fermions*.

Perhaps the most convincing macroscopic evidence that indeed there are heavy electrons in heavy fermion compounds comes from those materials that become superconducting. In a superconductor, there is a gap in the electronic spectrum at the fermi surface, and so the electronic specific heat disappears. Exactly that phenomenon is seen in experiment (Fig. E.5), so one can see that essentially all the low temperature specific heat is to be assigned to the carriers.

If one is confident that one has a metal, one can revisit the interpretation of



Figure E.4: . Specific heat of YbCuAl plotted in the form C/T vs. T^2 , which allows the electronic contribution to be read off by the asymptote.[Mattens et al , Comm. Phys. 2, 147 (1977)]



Figure E.5: . Specific heat of UBe_{13} at low temperatures. The normal state contribution is extrapolated through the superconducting transition at 0.9 K, and one can see that it is suppressed at low temperatures.[Ott et al., Phys. Rev. Lett. **50**, 1595 (1983)]



Figure E.6: . Resistivity of two heavy fermion compounds, $CeAl_3$ and $CeCu_6$. Note the sudden drop in resistivity at low temperatures as the systems become good metals. [Figure from G.R.Stewart, Rev.Mod.Phys. **56**, 755 (1984).]

the magnetic susceptibility. Pauli paramagnetism (Eq. (D.3)) gives

$$\chi_{\sigma} = \mu_B^2 g_{eff}(\mu) \quad . \tag{E.14}$$

Only if the mass is large, and density of states very high, can this be comparable to a Curie like term — remember that for a free electron gas

$$g_{eff}(\mu) = \frac{N}{V} \frac{3}{2E_F} \tag{E.15}$$

The pauli paramagnetism seen in metallic UPt_3 is as if the metal had a bandwidth of only tens of degrees K.

Resistivity

Nevertheless, it really is a metal. The resistivity in fact rises very slowly as the temperature is lowered, and the large resistivity reflects the fact that there is a high density of fluctuating spins to provide scattering; very abruptly at low temperatures, the resistivity drops as the susceptibility reaches its maximum. At low temperatures, the resistivity follows a T^2 law, $\rho = \rho_o + AT^2$, reflecting the fact that electron-electron scattering is growing rapidly with temperature on the scale of the very narrow bandwidth (see Fig. E.6). The T^2 power law reflects the lifetime of the quasiparticle near the fermi surface — according to fermi liquid theory $1/\tau = \Gamma \propto \max(\omega^2, T^2)$.



Figure E.7: . Fermi surface of UPt_3 as determined by fitting de Haas-Van Alphen measurements to a model bandstructure calculation. The observed bands match those described by both d- and f-electrons, and the effective masses for some bands are found to be very large. If it is assumed that the electrons are part of the core, the data does not match the band structure calculation. [Courtesy C. Bergemann et al.]

Fermi surface

The most convincing demonstration of the low temperature metal comes from the measurement of the fermi surface(s). Photoemission is not so easy to employ on such a narrow band system, because the energy resolution needed is extreme. A different approach is to make use of the behaviour of electrons in magnetic fields We have seen that the motion of a wavepacket is $\hbar \mathbf{k} = -e\mathbf{v}_{\mathbf{k}} \wedge \mathbf{B}$, namely the particle moves along an energy contour. If the fermi surface is closed, it will return to the same point periodically. Since electrons are quantum mechanical objects, we may guess that these orbits will be quantised, and the simple Bohr quantisation rule would say that the phase accumulated around the loop should be a multiple of 2π . The quantisation in a magnetic field will then give rise to magneto-oscillation phenomena, where physical properties oscillate as a function of 1/B with a prefactor that gives the *area* of the orbit, and can be used to determine cross-sections of the fermi surface perpendicular to the direction of magnetic field. When the measured quantity is the magnetisation, this is the de Haas-van Alphen effect, and an example of a fermi surface structure fit to dHvA experiments is shown in Fig. E.7.⁴ Analysis of the temperature dependence of the oscillations can be used to derive the effective masses.

 $^{^4{\}rm This}$ important experimental method will not be discussed here, but can be found in any major textbook. See Kittel, ch. 9 for example.

Recap of physical properties

Because this is real physics, the details vary somewhat from material to material, and there is some extra physics to describe on top of the basic scenario, but very roughly

Local moments. At high temperatures, there are seen to be dense local moments that give a Curie law in the susceptibility, Eq. (E.9).

Kondo temperature and coherence temperature. Around a temperature $T_K \approx \frac{1}{k_B \bar{g}} \exp(-1/\bar{g}J)$ the local moment from the f-level binds with the itinerant sea formed from the other lighter mass bands to make a non-magnetic singlet band. At this point the resistivity drops, the magnetic susceptibility saturates, and the specific heat becomes linear in T.

Heavy electrons. The metallic phase is described by a metal, with a susceptibility

$$\chi \approx \frac{N}{V} \frac{\mu_B^2}{k_B T_K} \quad , \tag{E.16}$$

and specific heat

$$C_{el} \approx \frac{N}{V} \frac{k_B T}{T_K} \quad . \tag{E.17}$$

This is just like a normal metal with a density of states

$$g_{eff} = \frac{N}{V} \frac{1}{k_B T_K} \tag{E.18}$$

Equivalently, this is an effective mass enhancement

$$\frac{m^*}{m} = \frac{g_{eff}(\mu)}{g(\mu)} \approx \frac{\text{bandwidth}}{k_B T_K}$$
(E.19)

that may be up to 10^3 .

Fermi surface. The fermi surface is as predicted by the bandstructure (i.e. including f-electrons as itinerant, not in the core), but the effective mass of the band is determined by Eq. (E.19), i.e. by the many-body hybridisation of the f-electron with the s-p-d bands — *not* by direct overlap of the orbitals.

Further properties.

This is far from the end of this subject, which remains an active field of research, and where there are many interesting unsolved issues.

Magnetic and/or orbitally ordered ground states. Although there was an implication that the magnetism entirely disappeared, this is not always the case, and many heavy fermion systems show weak (small moment) magnetic order at low temperatures - e.g. UGe_2 is a ferromagnet, $CePd_2Si_2$ is an antiferromagnet. In URu_2Si_2 a phase transition is seen at low temperatures



Figure E.8: (Phase diagram of UGe_2 under pressure. As the ferromagnetism disappears, there is a small window of superconductivity, surprisingly on the ferromagnetic side of the phase boundary. This is not understood - but conventional superconductors are made of singlet electron pairs and abhor magnetism. [Saxena et al. Nature **406**, 587, (2000)]

that opens a gap in the electronic spectrum, but where the form of the broken symmetry is not yet determined.

Unconventional superconductivity. Superconductivity is also often observed at low temperatures, and in several (possibly all) cases it is clear that the paired state is not the conventional s - wave symmetry of phonon-mediated superconductivity, but in general something more complex.

Quantum critical phenomena, and the breakdown of fermi liquid. Since the band-width is narrow, and the fermi energy is small, it is easy to apply external "fields" (e.g. magnetic field, pressure) that are energetically comparable to the fermi energy itself. These fields can often be enough to destroy one broken symmetry phase, and potentially reveal another. In the vicinity of the "critical point" (where the order parameter vanishes) there are soft, low energy quantum fluctuations that modify the physical properties of the metal, leading to anomalous — so-called "non-fermi liquid" behaviour. There is also much speculation that the soft magnetic fluctuations near the ferromagnetic transition are responsible for mediating superconductivity, for example.

Further reading

G.R.Stewart, *Heavy Fermion Systems*, Rev. Mod. Phys. 56, 756 (1984).
G.R.Stewart, *Non-fermi liquid behavior in d- and f- electron metals*, Rev. Mod. Phys. 73, 797 (2001).
A.C.Hewson, *The Kondo problem to heavy fermions*, (CUP, Cambridge, 1993).



Figure E.9: (Top) Intensity plot of the magnetic susceptibility of URu_2Si_2 measured in magnetic fields up to 40 T. The peaks mark phase transitions to states labelled 'HO' for " hidden order" and 'RHO' for " re-entrant hidden order", which indicates fairly accurately the current state of understanding of the underlying phases. (Bottom) Contour plot of the resistivity of the same material, suggesting even more complexity. [Kim et al, Phys. Rev. Lett. **91**, 256401 (2003)]