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Neutron-Electron Spectroscopy

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Abstract

Inelastic scattering of neutrons by electrons in a solid is an established technique by which to investigate processes that occur on a scale of energy up to about 0.2 eV, and the processes include spin-wave excitations and crystal-field states. The article looks at some examples of what can be gained from investigations conducted above this energy and up to several electron volts.

1. Orientation

The aim of this article is to stimulate, or possibly help renew, interest in the use of energetic neutrons to study properties of electrons in solids. To this end, we bring together basic features of the scattering of neutrons by electrons and look at what is expected if the electrons are localized in space (e.g. electrons in the f shell of a lanthanide ion) or mobile and band-like.

Of course, the use of thermal neutrons to study electrons in solids is very well established. Physical properties in this energy range include crystal-field states and collective spin excitations, often called magnons or spin waves.

There are at least two practical problems to be faced when it comes to using neutrons to investigate properties at higher energies, above about 0.2 eV; one problem, a sufficient supply of neutrons, in principle is largely resolved and the second, satisfying kinematics in an experiment, is handed down by Nature and we must learn to live with it. First, one needs a copious supply of energetic neutrons, and for these we turn to spallation sources. In the not too distant future, the supply will be very much improved by the operation of the Spallation Neutron Source under construction in Oak Ridge, USA (Mason et al. 2000) and perhaps also the AUSTRON source if the current project in Austria is brought to fruition (Rauch et al. 2000). Existing sources of energetic neutrons are more than adequate to make some measurements but new sources will surely open new vistas of research.

The second problem stems from the huge difference in the masses of the electron and the neutron. The challenge which then arises is to satisfy the twin objectives of a large transfer of energy, exceeding 0.2 eV, say, and only a modest change in the wavevector so as not to unduly suffer a shortfall in scattered intensity that will come about because of a monotonically decreasing form factor in the scattering length, which at a wavevector around $4\pi\text{Å}^{-1}$ might achieve a magnitude that is a few percent of its maximum value. With regard to this second problem one can realistically be optimistic about future activities because of what has been

achieved with existing instrumentation. In what follows, we do not dwell on the challenge to the experimentalist of detecting neutrons deflected through small angles.

The emphasis in this article is on processes that occur at an energy of about 0.2eV and beyond. In particular, we have little to say about crystal-field states even though they are an active field of research (Mesot 1995, Lovesey and Staub 2000, and Staub and Soderholm 2000).

2. **Neutron-electron interaction**

The contribution to the scattering length of the neutron due to its interaction with an electron has a size set by the classical radius of an electron, $r_e = \alpha^2 a_o = 0.282 \times 10^{-12}$cm, which is similar to the magnitude of many nuclear scattering lengths. Not surprisingly, the huge difference between the spatial sizes of a nucleus and an orbital for an electron in a solid leads to significant differences in the scattering profiles for nuclei and electrons.

There are two physically different components in the neutron-electron interaction. One is due to the spin of an electron and the second, quite often called the orbital interaction, is due to the magnetic field created by a moving charge. Hence, the interaction involves two degrees of freedom belonging to the electron, namely, its spin and its momentum (or velocity). The momentum can be re-expressed in terms the orbital motion of the electron, much as one does in a multipole expansion of a photon wave function to expose electric and magnetic absorption events. For elastic neutron scattering there is a one to one correspondence between the momentum-dependent interaction operator and orbital angular momentum; the correspondence was demonstrated by Trammell (1953) in a landmark paper. For inelastic scattering processes, of interest to us here, the correspondence is not one to one and, in fact, there is no benefit in using orbital angular momentum operators to describe truly mobile electrons. Instead, calculations of the cross-section, also called a profile, for itinerant electron systems are best done in terms of the linear momentum operator.

In discussing localized electron systems, we will not consider the algebra involved in relating the linear momentum operator to the orbital angular momentum operator for the algebra is quite involved (Balcar and Lovesey 1989) and a discussion of it adds little to the main aim of this article. Instead, we settle for quoting a result for the neutron-electron interaction operator for one ion expressed in terms of the total spin, **S**, and total orbital angular momentum, **L**, of the valence electrons (a matrix element of the interaction with electrons in core states is zero because electrons in these states are paired).

Restricting our attention, for the moment, to scattering events in which the primary beam is deflected through a modest angle the neutron-electron interaction operator is,

$$\mathbf{Q}(\mathbf{k}) = \tfrac{1}{2}[\{< j_o(k) > + < j_2(k) >\}\mathbf{L} + 2 < j_o(k) > \mathbf{S}]. \qquad (1)$$

Here, $\langle j_n(k)\rangle$ is a radial integral for electrons in the valence shell created by weighting the radial density of electron charge in the valence shell by the spherical Bessel function $j_n(kr)$ where k is the magnitude of the wavevector. It follows from the properties of $j_n(kr)$ that $\langle j_o(k)\rangle$ tends to a non-zero value as $k \rightarrow 0$, and it is customary to arrange normalization of the radial charge density such that $\langle j_o(0)\rangle = 1$. For n > 0 radial integrals evaluated with $k \rightarrow 0$ tend to zero. Hence, in the extreme limit of forward scattering (i.e. no deflection of the beam) the interaction operator (1) is proportional to the magnetic moment carried by the valence shell.

Let us consider a matrix element of (1) taken between states of different total angular momentum with quantum numbers J and J'. The situation $J \neq J'$ which we consider is realized by a scattering event that induces a transition between states with different J values in a multiplet, and between J-multiplets belonging to different term energies. The key result is that, non-diagonal matrix elements of the operator $\mathbf{J} = \mathbf{L} + \mathbf{S}$ are zero, and

$$< J \mid \mathbf{Q} \mid J' > = -\tfrac{1}{2} < J \mid \mathbf{L} \mid J' > \{< j_o(k) > - < j_2(k) >\}. \qquad (2)$$

The characteristic dependence of this matrix element on k is a signature of an inelastic event, and the dependence is quite different from that encountered with elastic scattering, e.g. Bragg diffraction.

To complete the present discussion let us consider the cross-section which arises from the result (2). Non-zero off-diagonal matrix elements of **L** must have $J' = J \pm 1$. Hence, for modest deflections of the beam inelastic events are subject to the dipole selection-rule. Consider $J = L + S$ and the event $J' = J - 1$ where the states labelled by J and J' are separated in energy by an amount Δ. The cross-section corresponding to this situation derived from (2) is found to be proportional to,

$$\frac{1}{6} r_e^2 \left(\frac{LS}{J}\right)\{< j_o(k) > - < j_2(k) >\}^2 \delta(\hbar\omega - \Delta), \qquad (3)$$

where $\hbar\omega$ is the change in energy of the neutrons; $\mathbf{k} = \mathbf{q} - \mathbf{q}'$ and $\hbar\omega = \hbar^2(q^2 - q'^2)/2m$ with $\hbar^2/2m = 2.072$ meVÅ^2. The result for $J = |L - S|$ and $J' = J + 1$ is very similar to this, of course, and the dependence on the atomic quantum numbers is a bit more complicated.

In general, the dipole selection rule does not limit the events observed in neutron-electron spectroscopy. The foregoing expressions actually refer to a very special case and experimental evidence for this is discussed later. For an arbitrary value of k there are no simple and general theoretical expressions for the cross-section, and each ion needs to be examined on an individual basis. Results for all the rare-earth (tripositive) ions are tabulated by Osborn et al. (1991).

As the last topic in the present discussion of inelastic scattering by an ion we wish to emphasize that, the intensity distribution as a function of k can be very different in inelastic and elastic scattering events. In the latter case the k-dependence of the scattering length is embodied in a so-called atomic form factor. To illustrate the difference in the k-dependence of intensity for inelastic and elastic events we show in Fig. 1 calculated results for Sm^{3+}. The inelastic event is dipole-allowed so the intensity for $k = 0$ is different from zero. The k-dependence of elastic scattering is unusual in so far that it is not monotonically decreasing, and this feature can be traced

to a near cancellation of the spin and orbital contributions of the magnetic moment which also leads to a small value of the gyromagnetic factor, namely, g = 2/7. The calculated elastic and inelastic structure factors displayed in Fig. 1 are in accord with experimental findings (Moon and Koehler 1979, Williams et al. 1987).

We next consider mobile electrons and find that the cross-section for inelastic scattering is likely to be profoundly different from results we have just discussed for localized electrons. One model we can treat completely is a gas of electrons which do not interact, the so-called ideal electron fluid or jellium model of electrons in a solid. Even though the Coulomb interactions between electrons, and between electrons and ion cores in the crystal are not included in the ideal electron fluid the electrons are correlated because of the quantum mechanical exchange force originating from the Pauli exclusion principle.

Since the electrons in the ideal fluid are identical and correlated it is not correct to consider scattering by a single electron. Instead, to calculate the profile one must employ a formalism that describes all electrons in the fluid on an equal footing and accounts for the Pauli exclusion principle. There are various ways of handling the calculation; perhaps the simplest is to use second quantization of the spin density and momentum density of the electrons. One finds that the cross-section is proportional to,

$$\frac{r_e^2}{n_o (2\pi)^3} \int d\mathbf{q} \{1 + \frac{2}{k^4} (\mathbf{k} \text{ x } \mathbf{q})^2\} f_{\mathbf{q}} (1 - f_{\mathbf{k+q}}) \delta[\hbar\omega + \varepsilon(\mathbf{q}) - \varepsilon(\mathbf{k} + \mathbf{q})]. \qquad (4)$$

In this expression, $f_{\mathbf{q}}$ is the Fermi occupation function for an electron with energy $\varepsilon(\mathbf{q}) = (\hbar q)^2/2m_e$ and n_o is the density of electrons. The expression (4) is the sum of contributions due to the spin and the orbital interactions, with the latter distinguished by the vector product $\mathbf{k}$ x $\mathbf{q}$.

The Fermi functions in (4) are a signature of quantum mechanics, and their influence is profound at low temperatures (the so-called degenerate Fermi fluid). One general feature that merits comment is the form of the cross-section for large values of

k. On taking the limit $k \to \infty$, the contribution from the orbital interaction is negligible and $f_{\mathbf{k+q}} \to 0$. The corresponding value of (4) is often referred to as the Compton limit of the cross-section, namely,

$$\frac{r_e^2}{n_o (2\pi)^3} \int d\mathbf{q}\, f_{\mathbf{q}} \delta[\hbar\omega + \varepsilon(\mathbf{q}) - \varepsilon(\mathbf{k}+\mathbf{q})]\,. \tag{5}$$

Although this result has been derived for ideal electrons, in fact, it is correct in the general case when $f_{\mathbf{q}}$ is the appropriate momentum distribution and the bare mass of the electron, m_e, is replaced by an effective mass.

Let us return to (4) and consider its behaviour in the limit of zero temperature. In this case,

$$f_{\mathbf{q}} = 1, |\mathbf{q}| < p_f \;:\; f_{\mathbf{q}} = 0, |\mathbf{q}| > p_f$$

where the Fermi wavelength p_f satisfies,

$$p_f = (3\pi^2 n_o)^{1/3}.$$

In the description of the profile it is quite convenient to use reduced variables for the energy transfer $x = \hbar\omega/\varepsilon_f$ and wavevector transfer $y = k/p_f$ where the Fermi energy $\varepsilon_f = (\hbar p_f)^2/2m_e$. Scattering is restricted to a domain in x–y space as a direct consequence of the Fermi functions. One finds the intensity profile for a degenerate ideal electron fluid is different from zero in the domain specified by the following conditions (the domain is often called the particle-hole continuum);

$$0 \le x \le (2y + y^2) : 0 \le y \le 2 \qquad (y^2 - 2y) \le x \le (y^2 + 2y) : y > 2.$$

The spin and orbital profiles, calculated from (4) with T = 0 K, p_f = 0.96 Å^{-1}, ε_f = 3.5 eV, and y = 0.57, are displayed in Fig. 2 as a function of $\hbar\omega = x\varepsilon_f$. Two features merit attention. First, the profiles extends over a wide range of energies and,

secondly, the orbital contribution exceeds the spin contributions. The latter feature is due to the factor $1/k^2$ in the orbital contribution to (4). In a real material and $k \rightarrow 0$ this contribution will saturate due to diamagnetic screening, for example.

3. **Intermultiplet transitions**

Fig. 3 shows experimental data collected on thulium metal at 20K. The incident neutron energy = 2.14 eV and the deflection of the beam = 5°. Calculations (Osborn et al. 1991) for tripositive thulium ion predict the lowest Coulomb transition $^3H_6 \rightarrow {}^3F_4$ at 693.5 meV, with transitions to the $^3F_3$ and $^3F_2$ levels at just under 2eV. Coulomb transitions, which are designated by $\Delta L \neq 0$, have energies that depend on the Coulomb repulsion between electrons in the valence shell. Since the Coulomb integrals are likely to be more sensitive to changes in the local environment than spin-orbit interactions, Coulomb transitions are a useful probe of the way intra-atomic correlations are influenced by forming the metallic state. There are strong deviations from the Landé interval rule because of intermediate coupling. Looking at Fig. 3, the Coulomb transition $^3H_6 \rightarrow {}^3F_4$ is lower in energy than the dipole-allowed transition $^3H_6 \rightarrow {}^3H_5$ and it is more intense. Measured and calculated intensities are gathered in Fig. 4. At a sufficiently small value of k the intensity of the dipole-allowed transition exceeds the intensities of all other transitions because these intensities vanish in the limit $k \rightarrow 0$.

Comparison of the transition energies for thulium metal, obtained by neutron-electron spectroscopy, with corresponding energies for thulium in LaF_3, obtained by optical studies, shows no appreciable differences. This finding suggests that for thulium metal there is no additional screening of the Coulomb interaction to that occurring in the isolated ion. A similar finding has been reported for $EuBa_2Cu_3O_x$ (x = 6.1 and 7) by Staub et al. (1997). There appears to be a more efficient screening of the Coulomb interaction by conduction electrons in Pr metal. Looking to the future, it will be valuable to measure the dependence on wavevector of structural factors for (intermultiplet) transitions split by the influence of the crystal field. Calculations (Staub et al. Private communication) using all the current

information on this material predict different dependencies for crystal-field split terms belonging to a multiplet.

Significant departures from isolated-ion behaviour can be expected in metallic systems where the 4f moment is inherently unstable. These include intermediate valence compounds, where two nearly degenerate electronic configurations are hybridized, and heavy-fermion compounds where the valence is nearly integral but strong band–4f hybridization suppresses the 4f moment. Similar phenomena are found in actinide compounds. In all cases, intermultiplet spectroscopy can provide valuable information, including the mixing of configurations and the degree of hybridization of the valence shell. A review of early work can be found in Osborn et al. (1991).

4. Neutron scattering from mobile electrons

As already mentioned, the physical processes we consider occur on an energy scale beyond about 0.2 eV. No experimental studies of mobile electrons in this domain of energy have been reported. In contrast, there is a multitude of studies of processes occurring at lower energies and, in particular, we have in mind the many studies of spin wave excitations in metallic systems.

Energetic neutrons might be used to conduct Compton scattering experiments. Because the scattering wavevector in these experiments is by design made very large the scattering is (spatially) incoherent. Results are essentially to do with individual particles and reveal nothing about spatial properties. The value of Compton scattering for studying the motion of nuclei in condensed matter is well established (Watson 1996 and references therein). We have seen that the Compton cross-sections for nuclei and electrons are the same; the information in them is to do with distributions in momentum space, and in the case of electrons the distribution in question is that of the spin density. The same physical information is available from the Compton scattering of x-rays, and many successful experiments using synchrotron sources have been reported (Sakai 1996).

Let us turn to the inelastic and coherent scattering of neutrons by mobile electrons. Our starting point is the discussion in section 3 of scattering by an ideal Fermi fluid. First, we consider the modification to this result brought about by switching on the Coulomb interaction between electrons. The plasmon is a collective oscillation in the density of electrons. The plasmon frequency at $k = 0$ is $\omega_p = (4\pi n_o e^2/m^*)^{1/2}$ where m* is the effective mass and some values calculated with $m^* = m_e$ are given in Table I. The dispersion of the plasmon is quite weak. For k beyond about p_f the plasmon is subject to strong damping from particle-hole states, which is also known as Landau damping.

The plasmon is invisible in neutron scattering, in zero applied field. The origin of this effect, essentially a selection rule, is orthogonality of the particle density that carries the oscillation and the spin density to which neutrons couple; the first density is $n\uparrow + n\downarrow$ and the second is $n\uparrow - n\downarrow$. Application of a magnetic field breaks the selection rule, and thereby a magnetic field is an excellent switch to use in picking out in the profile the contribution due to the plasmon.

Secondly, we look at the effect due to electron scattering by ion cores in a crystal on the spin and orbital profiles. Figs. 2 and 5 display profiles obtained from band-structure models of sodium and paramagnetic iron. In all the cases illustrated, spin underperforms orbital scattering. The unit of intensity used for the profiles is such that on multiplying by 0.29 the intensity is barns sr^{-1} eV^{-1}. (Noise arises in the profiles calculated from band-structure models from band degeneracies at the zone boundaries and the handling of the delta function that expresses conservation of energy, cf. (4).)

Fig. 2 includes profiles calculated for an ideal degenerate Fermi fluid. These are found to be a good guide for $\hbar\omega$ less than about 2 eV. Dramatic differences between results for the ideal fluid and band-structure models appear just above 3 eV. The origin of the distinctive features from the band-structure model is the splitting of the free electron degeneracy at the zone boundary, which is perpendicular to the (1, 1, 0) direction. This has been discussed extensively in the literature under the title of zone-boundary collective state.

An estimate of the profiles in terms of the density of electronic states $G(\varepsilon)$ can be obtained by averaging the cross-section over the directions of **k**. For the spin profile one arrives at,

$$r_e^2 \int_{-\infty}^{\infty} d\varepsilon \; f(\varepsilon)\{1 - f(\hbar\omega + \varepsilon)\}\, G(\varepsilon)\, G(\hbar\omega + \varepsilon)\,, \tag{6}$$

where $f(\varepsilon)$ is the Fermi occupation function for an electron with energy ε. The expression (6) has the form of a joint density of states. For simple metals ε_f is typically a few eV, as can be seen by reference to Table I. Hence, at room temperature it is appropriate to replace $f(\varepsilon)$ by a step function at ε_f, and in this case (6) reduces to,

$$r_e^2 \int_{o}^{\hbar\omega} d\varepsilon \; G(\varepsilon + \varepsilon_f - \hbar\omega)\, G(\varepsilon + \varepsilon_f) : \quad \hbar\omega < \varepsilon_f\,,$$

or (7)

$$r_e^2 \int_{o}^{\varepsilon_f} d\varepsilon \; G(\varepsilon)\, G(\varepsilon + \hbar\omega) \; : \quad \hbar\omega > \varepsilon_f \; .$$

In the limit $\hbar\omega << \varepsilon_f$ one obtains $r_e^2 \, \hbar\omega \, G^2(\varepsilon_f)$ as an estimate of the profile. The density of electronic states depends on the spatial dimension of the system. This observation leads one to anticipate that, cross-sections for highly anisotropic systems, which are quasi-one or –two dimensional, will be quite different from those featuring in Figs. 2 and 5.

For a 'top hat' electron density of states of total width ε_o the profile derived from (7) is zero except within an interval of energy between 0 and ε_0, where it is a triangle of height $(r_e^2 / 2\varepsilon_o)$. This finding indicates that scattering from mobile electrons is particularly intense for materials with a narrow band width.

Calculated spin and orbital profiles displayed in Fig. 5 are for a d-band metal, and the potential used in the band-structure calculation models paramagnetic iron. At the high energies of interest here enhancement of the spin response, required at low energies to reproduce the spin wave, is not significant and calculations reported in Fig. 5 contain no such enhancement. As noted already, the orbital outweighs the spin contribution to scattering. Another feature to note is the effect on a profile of increasing the magnitude of the scattering wavevector. In Fig. 5 the two panels correspond to wavevectors that differ by a factor = 4.3, while the scale for the intensity differs by an order of magnitude. Thus, increasing *k* reduces the signal from inelastic scattering by mobile electrons, and in this respect the scattering is not unlike intermultiplet transitions discussed in section 3. The cross-section to be observed in an experiment is the sum of the spin and orbital profiles separately displayed in Figs. 2 and 5.

Spin wave excitations in metallic systems continue to pose a major theoretical challenge, even elemental magnets, and there is a need for experimental investigations. For example, there remain basic questions about the spin waves in iron and nickel (Karlsson and Aryasetiawan 2000). Some calculations for nickel predict a spin wave branch that extends up to an energy of 0.5eV at the zone boundary, in addition to a softer spin wave that achieves half this energy. The dispersion, and temperature dependence, of the spin waves in nickel and other so-called simple metallic magnets are not understood and interplay between theoretical and experimental studies are much needed.

Magnetic materials very much at the centre of current research also support high-energy spin excitations. Measurements on La_2CuO_4 (Coldea et al. 2000) possibly include the most energetic excitations to have been observed. By using a spectrometer with many counters supplied with neutrons from a pulsed spallation source (the ISIS Facility), the investigators were able to convincingly demonstrate dispersion at the level of 10% in an excitation centred around 300 meV. This observation of dispersion has a very direct bearing on properties of the appropriate spin Hamiltonian.

5. Discussion

In bringing the article to a close it is fitting to add a few words about spectroscopic techniques applied to metals that utilize beams of x-rays. Synchrotron sources of x-rays developed over the past decade or so have made these techniques much more valuable than before (Margaritondo 1988).

X-ray absorption lineshapes and photoemitted electron energy distribution curves contain a wealth of useful information. The distribution curves measured in photoemission spectroscopy, for example, contain information on the initial electronic states and it appears in the curves convoluted and mixed with other effects that could be the prime interest. Effects in question include bulk and surface plasmons, secondary electrons from inelastic scattering processes, and the orthogonality catastrophe which is a many-body effect that arises with photoelectrons excited from core levels of an ion. The absorption of x-rays contains another many-body effect, namely, excitons which arise from the addition of electrons to the conduction band. Excitons and the orthogonality catastrophe cause power law behaviour at the absorption edge. Because of these and other effects measurements using x-ray spectroscopy are indeed rich in information content. On the other hand, the interpretation of data is both subtle and demanding, and very much more so than one anticipates with data gathered using neutron-electron spectroscopy.

One attraction of neutron-electron spectroscopy has to be the delicate nature of the neutron as a probe of condensed matter. The many-body effects in x-ray spectroscopy just mentioned are a measure of the disruptive nature of x-rays in this mode of investigation. If the goal of an experiment is to measure properties of electrons in the sample without a violent disturbance the method of choice is neutron-electron spectroscopy.

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References

Balcar E and Lovesey SW (1989) Theory of Magnetic Neutron and Photon Scattering (Clarendon Press: Oxford)

Balcar E and Lovesey SW (1993) J. Phys.: Condens. Matter **5**, 7269

Blackman JA et al. (1987) J. Phys. C: Solid State Phys. **20**, 3887
ibid **20**, 3897

Coldea R et al. (2000) Physica B **276** – **278**, 592

Karlsson K and Aryasetiawan F (2000) J. Phys.: Condens. Matter **12**, 7617

Lovesey SW and Staub U (2000) Phys. Rev. **B61**, 9130

Margaritondo G (1988) Introduction to Synchrotron Radiation (Oxford University Press : New York)

Mason TE et al. (2000) Proceedings of the LINAC 2000 Conference, paper FR203

Mesot J (1995) in Magnetic Neutron Scattering edited by A Furrer (World Scientific: Singapore)

Moon RM and Koehler WC (1979) J. Mag. & Mag. Mat. **14**, 265

Osborn R et al. (1991) in Handbook on the Physics and Chemistry of Rare Earths, Vol. 14, Chapter 93 (Elsevier Science Publishers: Amsterdam)

Rauch H et al. (2000) Physica B **276**-**278**, 33

Sakai N (1996) J. Appl. Cryst. **29**, 81

Staub U et al. (1997) Phys. Rev. **B55**, 11629

Staub U and Soderholm L (2000) in Handbook on the Physics and Chemistry of Rare Earths, Vol. 30, Chapter 194 (Elsevier Science Publishers : Amsterdam)

Trammell GT (1953) Phys. Rev. **92**, 1387

Watson GI (1996) J. Phys.: Condens. Matter **8**, 5955

Williams WG et al. (1987) J. Phys. **F17**, L151

Figure Captions

Fig. 1. Calculated structure factors for Sm^{3+}, showing the significant differences to be found for elastic and inelastic (dipole-allowed) events.

Fig. 2. Spin and orbital profiles for scattering from mobile electrons. Smooth dotted curves are derived from the spin and orbital contributions to (4). The reduced wavevector $y = 0.57$, and for this relatively small value the orbital contribution exceeds the spin contribution. The full and broken curves are the spin and orbital contributions obtained from a band-structure model of sodium and $\mathbf{k} = (¼, ¼, 0)$ in units of $(2\pi/a) = 1.55Å^{-1}$. Results are taken from Blackman et al. (1987).

Fig. 3. Neutron scattering cross-section for thulium metal showing intermultiplet transitions from a ground state $^3H_6$. The peaks are labelled by the final state of the transition. After Osborn et al. (1991).

Fig. 4. Inelastic structure factors for intermultiplet transitions in thulium. Experimental data is obtained from spectra such as the one displayed in Fig. 3, which is taken at an angle = 5°; $^3F_4$ filled circles, $^3H_5$ filled triangles, $^3H_4$ open circles and $^3F_3$ filled squares. The continuous curves are results obtained from theory based on an isolated ion. After Osborn et al. (1991).

Fig. 5. Calculated spin and orbital profiles obtained from a band-structure model of paramagnetic iron (Blackman et al. 1987). In the upper panel $\mathbf{k} = (½, ½, 0)$ and the bottom panel $\mathbf{k} = (3, 0, 0)$ and the unit is $(2\pi/a) = 2.3Å^{-1}$. For $k = 1.6Å^{-1}$ (upper panel) and $k = 6.9Å^{-1}$ the spin profile (solid curve) is weaker than the orbital profile.

Table I

The density of an electron gas and r_s are related through,

$$\frac{4\pi}{3} r_s^3 = \frac{1}{n_o a_o^3} ,$$

where a_o is the Bohr radius. In units of eV, the Fermi energy and plasmon energy are, $\varepsilon_f = 50.13/r_s^2$ and $\hbar\omega_p = 47.15/r_s^{3/2}$, and $p_f = (\varepsilon_f/3.80)^{1/2}$ Å^{-1}.

Metal	r_s	p_f (Å^{-1})	ε_f (eV)	$\hbar\omega_p$ (eV)
Li	3.24	1.12	4.78	8.08
Rb	5.23	0.69	1.83	3.94
Zn	2.30	1.58	9.48	13.52
Al	2.07	1.75	11.70	15.83
Sn	2.22	1.63	10.17	14.25