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# LOCAL SPIN DENSITY THEORY FOR FERRO-AND ANTIFERROMAGNETIC MATERIALS

N. E. Christensen, O. Gunnarsson, O. Jepsen and O. K. Andersen

Max-Planck-Institut für Festkörperforschung, Postfach 80 06 65, D-7000 Stuttgart 80, F.R.G.

Abstract. – The application of the density-functional theory in the local approximation to magnetic materials is discussed and illustrated by examples. The magnetic properties of the 3d elemental metals as well as their cohesive properties are described by means of self-consistent local-spin-density (LSD) calculations and by using the LSD-Stoner method. The application of the LSD approximation to narrow-band compounds (3d-monoxides) and to lanthanum cuprate indicates that correlation effects beyond those included in the LSDA must be added in order to obtain a realistic description of the ground state. The LSDA fails in predicting the antiferromagnetic ground state of  $La_2CuO_4$ .

#### 1. Introduction

A quantum-mechanical treatment of the electron states in a solid requires methods that can handle true many-body systems. Such theories are well explored for a uniform electron gas, but in order to be able to treat real materials, they must be extended to the case of an inhomogenous electron distribution. Simultaneously, the wish of performing actual numerical calculations of microscopic and macroscopic physical properties requires that the theory can be simplified so much that it can be implemented in a reasonably sized computer. This important goal of solid state theory appears very ambitious, but much progress has been made in that direction. There are three developments that have contributed decisively in achieving this. Firstly, the density functional (DF) theory [1, 2], including its local approximation [2] demonstrated how the many-electron problem can be transformed into an effective one-particle problem. Secondly, the development of computers allowed fast, numerical calculations. Thirdly, the advent of new, efficient schemes for selfconsistent band structure calculations, such as, for instance, the linear methods [3, 4], allowed the very extensive tests and applications of the quantum theory of the solid state performed during the last decade.

Most of the work in the DF formalism has been based on a very simple approximation, the local (spin) density approximation (L(S)DA). It has been used to study many properties of atoms, molecules, and solids with an accuracy which by far exceeds the original expectations. During the last few years it has become costumary to discuss the cases where the LDA (LSDA) fails rather than its wellknown successes. We shall also, to some extent, follow this line, and comment on some of the systems for which the LSDA seems not to work well, "Mott insulators" and (maybe) 3d transition metals. The DF theory is designed to calculation of ground state properties, and not excitation spectra [5]. Thus, a disagreement with optical spectroscopy is not necessarily a real "failure", while a wrong prediction of the ground state, structure, magnetism shows that the approximations made in the actual calculation are not sufficiently accurate for the case considered.

#### 2. Density-functional theory and LSDA

In the DF formalism of Hohenberg Kohn and Sham [1, 2] ground state energy of a system in an external potential  $v_{\text{ext}}$  is written as

$$E[n] = T_s[n] + \int \left[\frac{1}{2}\int \frac{2n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}d\mathbf{r}' + v_{\text{ext}}(\mathbf{r})\right]n(\mathbf{r})d\mathbf{r} + E_{\text{xc}}[n(\mathbf{r})], \quad (1)$$

where  $T_s[n]$  is the kinetic energy of noninteracting electrons with the density  $n(\mathbf{r})$ , and  $E_{\mathbf{x}\mathbf{c}}[n]$  is the exchange-correlation energy. E[n] is minimized by the correct ground-state density. The minimization of equation (1) leads to the one-particle equation

$$\left[-\nabla^{2}+v_{\text{eff}}\left(\mathbf{r}\right)\right]\psi_{j}\left(\mathbf{r}\right)=\varepsilon_{j}\psi_{j}\left(\mathbf{r}\right),$$
(2)

and the density is

$$n(\mathbf{r}) = \sum_{j}^{\text{occ}} |\psi_j(\mathbf{r})|^2.$$
(3)

The effective potential is given by

$$v_{\text{eff}}(\mathbf{r}) = \int \frac{2n(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + v_{\text{ext}}(\mathbf{r}) + \frac{\delta E_{\text{xc}}[n(\mathbf{r})]}{\delta n(\mathbf{r})}.$$
(4)

In this way the many-body problem is mapped onto an equivalent one-particle problem. The exchangecorrelation functional is unknown, but the *local* approximation:

$$E_{\rm xc} \approx \int \varepsilon_{\rm xc} \left[ n\left( {\bf r} \right) \right] n\left( {\bf r} \right) {
m d}{f r},$$
 (5)

where  $\varepsilon_{\rm xc}$  is the exchange plus correlation energy per electron in a homogenous electron gas of density  $n_0 = n(\mathbf{r})$ , has been very successful, not only because of its simplicity, but also because the actual numerical results obtained are realistic. Including the spin, we express the total density as  $n = n_{\uparrow} + n_{\downarrow}$ , and the spin density as  $m = n_{\uparrow} - n_{\downarrow}$ . In the LSDA the exchange-correlation part of the effective potential then becomes,

$$\mu_{\mathbf{x}c\sigma}\left(\mathbf{r}\right) = \mathrm{d}\left[\left(n_{\uparrow} + n_{\downarrow}\right)\varepsilon_{\mathbf{x}c}\left(n_{\uparrow}, n_{\downarrow}\right)\right] / \mathrm{d}n_{\sigma}.$$
 (6)

Actual forms may be found in references [6, 7]. To first order in m (see for example Ref. [8]),

$$\mu_{\mathrm{xc}\downarrow\uparrow} = \mu_{\mathrm{x}} \left[ \beta \left[ n \left( \mathbf{r} \right) \right] \pm \frac{m \left( \mathbf{r} \right)}{3n \left( \mathbf{r} \right)} \delta \left[ n \left( \mathbf{r} \right) \right] \right], \qquad (7)$$

where  $\mu_x$  is the Kohn-Sham exchange potential evaluated at the density  $n(\mathbf{r})$ . Other approximations for the exchange and correlation effects have been given by Gunnarsson *et al.* [9] and Langreth, Mehl and Hu [10]. The external potential appearing in the Schrödinger like equation (the Kohn-Sham Eq. (2)) consists in a solid of the potential from the nuclei. If a magnetic field, is applied, it should also include a term  $-\text{sign}(\sigma) \mu_B H$ . With the  $\uparrow, \downarrow$  exchange-correlation potentials (7) it follows that for a para- or ferromagnet the K-S equation separates into two, one for each spin direction.

2.1 LDA STONER THEORY OF FERROMAGNETISM. – It has been demonstrated that a simple Stoner theory can be derived within the DF formalism [11, 8, 12], and that it gives a quite accurate description of the magnetic properties of the alkali [11] and ferromagnetic 3d [8, 13] metals. We introduce a Stoner parameter Iwhich describes the spin splitting of the states,

$$\Delta \varepsilon \left( j, \mathbf{k} \right) = \varepsilon_{j\downarrow}^{\mathbf{k}} - \varepsilon_{j\uparrow}^{\mathbf{k}} = 2 \ \mu_{\mathrm{B}} H + m I \left( j, \mathbf{k} \right), \qquad (8)$$

where, to first order in the relative magnetization density,  $m(\mathbf{r}) / n(\mathbf{r})$ ,

$$I(j,\mathbf{k}) = -\left\langle \psi_{j}^{\mathbf{k}} \middle| \frac{2\delta[n(\mathbf{r})]\,\mu_{\mathbf{x}}[n(\mathbf{r})]\,m(\mathbf{r})}{3n(\mathbf{r})\,m} \middle| \psi_{j}^{\mathbf{k}} \right\rangle. \tag{9}$$

If the wavefunctions at the Fermi surface have only one dominating angular-momentum component (l), and if the spin densities are spherically symmetric inside Wigner-Seitz spheres of radius s (atomic-spheres approximation (ASA) I is given by the approximate expression [8, 12]:

$$I \approx -\int_{0}^{s} \frac{\delta[n(r)] \,\mu_{\mathbf{x}}[n(r)]}{6\pi n(r)} \phi_{l}^{2}\left(\varepsilon_{j}^{\mathbf{k}}, r\right) \phi_{l}^{2}\left(\varepsilon_{\mathbf{F}}, r\right) r^{2} \mathrm{d}r,$$
(10)

which is merely energy- rather than state dependent. There are several calculations of the Stoner parameter [11, 8, 14, 15]. In figure 1 we show the results [16, 14] for I (9) averaged over the (paramagnetic) Fermi surface. At the beginning of the transition series I decreases with increasing number of valence electrons, N,



Fig. 1 – The Stoner parameter calculated from LMTO wavefunctions (from Ref. [16]).

due to the factor  $\mu_x(\mathbf{r}) / n(\mathbf{r}) \sim N^{-2/3}$ . At end of the series this effect is overshadowed by the contraction of the predominantly d-like wave function entering with the power 4 (10).

The electronic structure corresponding to the simplified scheme defined by equations (8) and (10) has  $\uparrow$ - and  $\downarrow$ -density-of-states (DOS) functions which have the same *shape* (but not necessarily the same widths), and they may be derived from the non-spin-polarized DOS,  $N(\varepsilon)$  (per spin). The magnetization may be obtained from the Stoner-like equation [12]:

$$I\tilde{N}(m) = 1, \tag{11}$$

where  $\bar{N}(m) (\equiv m / (\varepsilon_{\uparrow}(m) - \varepsilon_{\downarrow}(m)))$  is the DOS averaged between the energies  $\varepsilon_{\downarrow}(m)$  and  $\varepsilon_{\uparrow}(m)$  defined by:

$$\frac{1}{2}m = \int_{\epsilon_{\rm F}}^{\epsilon_{\uparrow}(m)} N(\varepsilon) \,\mathrm{d}\varepsilon = \int_{\epsilon_{\downarrow}(m)}^{\epsilon_{\rm F}} N(\varepsilon) \,\mathrm{d}\varepsilon.$$
(12)

The derivation of the moment is illustrated in figure 30 of [16] for bcc iron, and the method has been applied in conjuction with the canonical band theory that emerges from the LMTO scheme, to examine [13, 14] metamagnetic behaviour of for iron. The magnetic energy contribution is,

$$E_m = \frac{1}{2} \int_0^m \frac{m' \mathrm{d}m'}{\bar{N}(m')} - \frac{1}{4} I m^2, \qquad (13)$$

and sationary solutions are found by requiring  $\partial E_m / \partial m = 0$ , yielding (11). The solution is obtained if  $\partial^2 E_m / \partial^2 m > 0$ , i.e. if  $\partial \overline{N}(m) / \partial m < 0$ . We have used [17] this Stoner model to study in detail the ferromagnetic phases of fcc Fe as a function of volume (Wigner-Seitz radius s). In figure 2 we show the graphic determination of the moment at a volume corresponding to s = 2.70 bohrs. For this purpose (11) is used in the form  $W_d(\varepsilon) N(m) = W_d(s) / I$ , where  $W_d(s)$  is the d-band width, because then the function



Fig. 2. – Iron, fcc, s = 2.70 a.u. Stoner criterion based on DOS functions (paramagnetic) calculated by the LMTO method in conjunction with LDA. Dashed arrows indicate unstable solutions, whereas LS1, LS2 and HS are the stable low-spin and high-spin solutions (Ref. [17]).

on the left-hand side is essentially volume independent, and the right-band side has approximately the volume dependence of  $W_d(s) \propto s^{-5}$ . It is seen, that three stable solutions, two low-spin (LS2 and LS1), and one high-spin (HS) phase, are predicted. The volume ranges where these phases are stable are shown in figure 3. There are ranges where three magnetic phases may coexist. It is obvious that the details of the phase diagram are related to the structure in the  $\bar{N}(m)$  – function, which in turn depends sensitively on the crystal structure. Thus, bcc Fe, for instance, has a completely different phase diagram [12]. The results figure 3 agree with those obtained by Moruzzi et al. [18, 19]. The fully self-consistent spin-polarized calculations by Kübler [20] only showed two magnetic phases in fcc Fe. Although the scf LSDA calculations



Fig. 3. – Fe (fcc). Stationary magnetic moment as a function of the atomic-sphere radius s. The branches indicated by a full line are stable, the dashed portions refer to unstable solutions. The non-magnetic state is stable (m = 0)up to the point (s = 2.706 a.u.) where the lowest unstable branch begins.

are very useful, in particular when used in the "fixedmoment" mode [18], an examination of the magnetic behaviour is more conveniently carried out by means of the Stoner analysis, as illustrated here for fcc Fe. This is also demonstrated by the study of the 3d metals by Moruzzi and Marcus [21]. They examine the magnetic phases by expanding the lattice from volumes below the observed equilibrium, beyond the onset of ferromagnetism and towards the atomic limit, and find that all 3d transition metals from Sc to Ni undergo secondorder, first-order, or composite second- and first-order transitions from nonmagnetic to magnetic phases.

While the LSDA-Stoner theory usually describes T = 0 properties well, those at finite temperatures are unsatisfactory. Thus, Gunnarsson showed [8] that it leads to far too large values of the Curie temperature,  $T_{\rm C}$  of the order of 5000 K for Fe and 2900 K for Ni. Oles and Stollhoff [22] argued that the LSDA underestimates the correlation effects, and adding the correlation as given in their local-ansatz approach they obtained lower values of the exchange splittings and better values of  $T_{\rm C}$ , 2560 K and 1790 K for Fe and Ni, respectively. These are still much larger than observed, 1068 (Fe) and 759 K (Ni). Mohn and Wolfarth [23] demonstrated that spin fluctuations in the form described by Lonzarich and Taillefer [24] provide an additional lowering of  $T_{\rm C}$ , and their quantitative results, 1068 (Fe) and 656 K (Ni), agree extremely well with experiments. A somewhat different approach was used by Gyorffy et al. [25] and by Lichtenstein et al. [26].

2.2 LSDA SCF CALCULATIONS. - The simple LDA-Stoner formalism discussed in the preceeding section uses spin-restricted density-of-states functions. Nearly all existing LSDA calculations are, however, fully selfconsistent in the spin polarization, and the Stoner formalism is usually used to interpret the results. In this way a higher degree of precision than can be obtained than with the approximations made in the LDA-Stoner scheme. This is in particular important for the calculation of structural energy differences which are, in some cases, minute. Moruzzi et al. [19] compare for Fe the total energies of bcc-ferromagnetic (F), fccnonmagnetic (N) and fcc-F phases. It was found, as we already saw in the previous section, that fcc-F only exists for expanded volumes, and; in agreement with experiment, that bcc-F has the lowest total energy at zero pressure. Using the LMTO method we [27, 17] found total-energy variations very similar to those shown in figure 9 of reference [19], provided that we include only s-, p-, and d-partial waves. Extending, however, the basis set to include f-partial waves we obtained the total energies as displayed in figure 4. Now the fcc-N clearly has a lower minimum energy than bcc-F (where the moment is 2.13  $\mu_{\rm B}$ ). This is not an artefact of the ASA functional; a similar result was obtained by Wang et al. [28] by means of the general-



Fig. 4. – Total energies calculated by means of the LMTO methd using the LSDA, and including s-, p-, d-, and f-partial waves, for bcc-P, bcc-F and fcc-P iron (F for ferro-, P for paramagnetic). The total energies of the fcc-F phases appearing for s > 2.64 a.u. are not shown.

potential LAPW method. This calculation further predicted an fcc antiferromagnetic (AF) phase to have the same minimum energy as fcc-N (see also Ref. [20]). These results are now taken as an indication of a failure of the LSDA in predicting the ground-state crystal structure, but it may merely be a manifestation of the well-known fact that the LDA generally overestimates the binding, e.g. the LDA equilibrium volumes are too small. The LDA total energy thus seems to be missing a term which decreases with volume, and which is essentially independent of structure. LDA calculations isoelectronic elements Ru and Os yield pressures of about -100 kbars at the experimental lattice constants. If we take this to give the order of magnitude of the volume dependence of the missing energy term and add this to all the curves in figure 4 we do find that bcc-F, rather than fcc-P, is now the stable phase, and that its equilibrium volume is now correct. Preliminary calculations using the non-local functional of reference [10] also indicate that it is the LDA overbinding which is mainly responsible for the prediction of the wrong ground state of iron.

In reference [29] we examine the ground-state properties of Ni-hybrides as a function of hydrogen content. The decrease of the saturation magnetisation with increasing H-concentration predicted by these scf LSDA calculations agrees with experiment. Also the volume expansion, which saturates at  $\approx 75$  at. % H, is well described by the theory. Selfconsistent LSDA calculations are in progress for compounds of Fe and lanthanides (e.g. TbFe<sub>2</sub> [30]) as well as Fe-actinide compounds [31]. These compounds have important technological applications (magneto-optic recording). Calculation of their magneto-optic effects requires the simultaneous inclusion of spin-orbit coupling and spin polarisation. Such calculations, based on a fully relativistic, spin-polarized LMTO, method, are described by Ebert *et al.* [32] and by Lichtenstein and Antropov [33]. Fritsche *et al.* [34] include spin-orbit coupling in general potential LAPW calculations for ferromagnetic thin films in order to obtain magnetic anisotropy energies.

2.3 Mott insulators and high- $T_c$  materials. – The electronic properties of the monoxides MnO, FeO, CoO, and NiO, have been the subject of many, and controversial, discussions. They are usually considered as being Mott insulators [35], or to be classified according to a generalized version of the Mott theory [36]. A description of the theory derived from Mott's arguments may be found in the review by Brandow [37] and more recently by Zaanen and Sawatzky [38]. In conventional band theory these oxides would be metals, although Slater [39] suggested that magnetic effects (antiferromagnetism) could create a gap in NiO. Andersen et al. [40] demonstrated that if antiferromagnetism is taken into account, then the LSDA describes the reduced cohesion and the correspondingly large lattice parameters of these systems. Recently the LSDA calculations by Terakura et al. [41] have revived the discussion about the "Mott-Hubbard" theory versus "band" theory. The LSDA calculation of reference [41] shows that NiO indeed in this approximation has an antiferromagnetic, insulating ground state. The gap, however, is very small,  $\approx 0.3$  eV. Photoemission and bremsstrahlung isochromat spectroscopy data indicate [42] a large gap, 4.3 eV. Norman and Freeman [43] argue that the LSDA band structure should not be related to the experiments of reference [42], and they show that excitation spectra derived from a supercell calculation where the localised hole of the excied state is treated as an "impurity" leads to good agreement with the experiment.

The ground state of the "mother material" of high-temperature superconductors, La<sub>2</sub>CuO<sub>4</sub>, is antiferromagnetic with a moment of  $0.4 \mu_B$ , but LSDA calculations [44] fail to yield this. The effective Stoner parameters turns out to be at least a factor 5 too small as derived from LMTO-ASA [3] calculations. The effect of going beyound the ASA, i.e. avoiding the spherical averaging of the spin density, has been estimated [44] to increase Iby at most a factor 2. Thus, in that case the LSDA cannot predict the correct ground state. The strength of the correlations not included in the LDA has been estimated by Oles et al. [45] and Fulde [46] using the local-ansatz method [22], and it was shown that they cause a small shift in the charge distribution; the d count  $n_d = 9.5$  in the independent-electron scheme changes to 9.3 when correlation is included. In the independent-particle picture the probabilities of finding the Cu-  $d^{10}$ -,  $d^9$ -,  $d^8$ configurations are [45, 46] 0.56, 0.38, and 0.06, respectively. With correlations the values are 0.29, 0.70, and 0, showing that the  $d^8$  configuration now is totally suppressed. A similar analysis for the oxygen atoms shows [46] that the  $2p^4$  configuration is *not* suppressed, and this may be important in establishing an antiferromagnetic coupling of the Cu sites. An improved LSDA formalism where self-interaction corrections (SIC) are included have been applied in a model calculation [44] for the CuO<sub>2</sub> planes in lanthanum cuprate, and this leads [47] to an antiferromagnetic solution with a moment of 0.6-0.8  $\mu_B$ . Application of a pure LSDA calculation to the same system yields a (almost) vanishing moment.

In view of these examples, which demonstrate shortcomings of the LDA it was very surprising to find [48] that the Fermi surface calculated within the LDA for the heavy-electron system UPt<sub>3</sub> agrees extremely well with the experimental de Haas-van Alphen data, although very strong correlation effects are omitted in the theory. As discussed elsewhere [49] this observation presumably reflects that in UPt<sub>3</sub> the crystalfield splitting is small, even compared to the width of the renormalized U-f(j = 5/2) band, and the spinorbit splitting is large as compared to the LDA width of the U f-band. The first of the conditions is not satisfied in CeAl<sub>3</sub>, and thus in that case we would not expect the LDA Fermi surface to agree with experiments. CeSn<sub>3</sub>, on the other hand, has a much larger f-band width, and the criteria above are fulfilled, and indeed the LDA Fermi surface seems to correspond well to the experimental data.

We have summarized many results showing that the LDA does not account properly for correlation effects in narrow-band materials. This does not imply that LDA (LSDA) calculations for these systems are useless. Several works have shown that they provide a convenient tool for obtaining [50] parameters of model Hamiltonians which explicitly include correlations such as the Anderson [51] impurity Hamiltonian. Earlier, these parameters were obtained by relatively crude estimates, or by fitting to experimental data. The direct calculation of the Anderson parameters may prove fruitfull in the theoretical studies of the high- $T_c$ superconductors (see, for example Refs. [52, 44, 53]).

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