# Magnetic susceptibility and spin waves in ferromagnetic metals

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The transverse magnetic susceptibility of a ferromagnetic metal is studied within the framework of the local-density approximation. An expression is derived for the wave-vector- and frequency-dependent susceptibility matrix which does not contain explicit reference to the exchange-correlation potential. This result leads to an explicit formula for the spin-wave stiffness, which is evaluated for nickel.

# I. INTRODUCTION

This paper is the first of a (projected) series dealing with the magnetic susceptibilities of ferromagnetic transition metals within the framework of the local-density approximation. In this paper, we will present a new expression for the transverse susceptibility matrix from which the spin-wave stiffness constant can be derived, and report the results of the evaluation of the latter quantity for nickel. Subsequent articles are intended to present results of numerical calculations of wave-vector and frequency-dependent susceptibility matrices.

In a fundamental paper, Izuyama, Kim, and Kubo<sup>1</sup> obtained expressions for the cross section for neutron scattering by a ferromagnetic metal in terms of wave-vector and frequency-dependent susceptibilities, which could be evaluated given the electron energy bands and wave functions. The susceptibility has poles at the energies of spin-wave modes, and an important contribution of their work was the development of a procedure for the determination of spin-wave energies, leading to an explicit expression for the spin-wave stiffness coefficient in terms of first and second derivatives of the band energies.

Izuyama, Kim, and Kubo applied the randomphase approximation (RPA) to the simplest form of Hubbard model: a short-range interaction in a simple tight-binding band. This work has been extended by many authors. Two major directions of subsequent research can be distinguished: (1) refinements of the techniques of many-body theory employed, and (2) extensions of the band model to enable a more realistic description of a real metal.

The practical use of the Hubbard model requires parametrization of the electron interaction. Since real transition metals are many band systems, several parameters are required—and these can only be estimated rather crudely. The situation is complicated by the fact that band calculations normally include some description of electron interactions at the level of a self-consistent field. The proper treatment of electron interaction corrections must first separate out that portion of the interaction which is included in the band calculations.

We have observed elsewhere<sup>2,3</sup> that the localdensity approximation contains enough of the electron interaction so that from a self-consistent calculation of the susceptibility, spin-wave energies can be directly determined without introducing any additional parametrization of the interaction. Our objective in this and the following papers is to investigate the extent to which quantitative results are in agreement with experiment. In this way, we expect to develop understanding of the range of accuracy and of the applicability of the local-density approximation.

In a pioneer calculation, Lowde and Windsor<sup>4</sup> studied neutron scattering from nickel on the bases of a simple tight-binding model of the energy band structure and a Hubbard model of the electron interaction. A momentum-dependent effective interaction was introduced. Calculations were made over a range of temperatures from  $0.5T_c$  to  $1.9T_c$ . They were able to reproduce many of the essential qualitative of the observed neutron scattering cross sections.

The approach of Lowde and Windsor has been extended to more realistic band-structure models in an extensive series of computation summarized recently by Cooke, Lynn, and Davis.<sup>5</sup> These authors retain the band and wave-vector dependence of the matrix elements relevant to the calculation of the susceptibility. A RPA treatment of the electron interaction is employed. They retain only two constants to describe this interaction, which are, essentially, diagonal matrix elements of a self-consis-

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tently screened potential, referring to states of  $t_{2g}$ and  $e_g$  symmetry. These quantities can differ significantly: In nickel, Cooke *et al.* propose that the exchange splitting of  $t_{2g}$  states is 0.4 eV, while that of  $e_g$  states is much smaller, 0.1 eV. This makes the generation of a semiempirical spin polarized band structure possible, which is in reasonable agreement with recent photemission measurements.<sup>6,7</sup> However, in iron, the exhange splitting of the  $t_{2g}$  and  $e_g$  states does not differ significantly. In a calculation restricted to T=0, Cooke *et al.* find spin-wave dispersion relations for both iron and nickel which are in good agreement with experiment. Optical spin-wave modes are also predicted.

In contrast to these calculations, we will use just the description of the electron interaction that is contained in the self-consistent band calculation. It must be noted that in the case of nickel, the band calculations<sup>8</sup> have an exchange splitting which is larger than that deduced from photoemission experiments. However, for iron substantial agreement between the calculated band-structure<sup>9</sup> and photoemission experiments<sup>10</sup> seems to exist. Our approach leads to an expression for the transverse susceptibility which does not make explicit reference to the electron interaction (it is, however, contained in the energies and wave functions). This result may have some usefulness beyond the boundaries of our specific calculation.

The self-consistent method leads to a general expression from which spin-wave energies and widths may be obtained. Explicit results have been obtained for the spin-wave stiffness.<sup>11-13</sup> Our preliminary numerical result for this quantity (in the case of nickel)<sup>11</sup> has turned out to be incorrect because of an error in the computer program. A revised value is reported in this paper.

### **II. FORMULA FOR THE SUSCEPTIBILITY**

We begin with an apparently single-particle Hamiltonian  $H_0$  which contains an exchangecorrelation potential  $V_{xc,\sigma}$ , which depends on the electron-spin densities  $\rho\sigma$ . We will use the notations  $\rho_t$  and  $\rho_{\downarrow}$  to designate the densities of electrons of majority and minority spins, respectively, in the ground state of the ferromagnet. The term "apparently single particle" is intended to describe a situation in which there is an effective Hamiltonian for single particles which depends on the charge and spin densities of all particles, and so contains in fact a partial description of the electron interaction at the level of a self-consistent field.

We write the Hamiltonian in the form

$$H = \frac{p^2}{2m} + V_0(\vec{r}) + V_f(\vec{r})\vec{\sigma}\cdot\hat{n} , \qquad (2.1)$$

in which  $V_0$  contains the Coulomb potential, and the spin average of  $V_{\rm xc}$ 

$$V_{0}(\vec{r}) = -\sum_{\mu} \frac{Z_{\mu}e^{2}}{|\vec{r} - \vec{R}_{\mu}|} + e^{2} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^{3}r' + \frac{1}{2} [V_{\text{xct}}(\vec{r}) + V_{\text{xct}}(\vec{r})]. \qquad (2.2)$$

In this expression the nuclei of the system are located at sites  $\vec{R}_{\mu}$  and have charge  $Z_{\mu}$ ,  $\rho$  is the total electronic charge density, and the last term represents the spin average of the exchange-correlation potential. The last term in (1) contains  $V_f(\vec{r})$ , which is given by

$$V_f(\vec{\mathbf{r}}) = \frac{1}{2} \left[ V_{\text{xc}\dagger}(\vec{\mathbf{r}}) - V_{\text{xc}\downarrow}(\vec{\mathbf{r}}) \right], \qquad (2.3)$$

 $\sigma$  is the usual Pauli spin operator, and  $\hat{n}$  is a unit vector in the direction of the magnetization of the material. The explicit form of  $V_{\rm xc}$  is not relevant until numerical calculations are discussed.

The calculations of spin-wave energies in this procedure follows from the transverse susceptibility. This is determined by a self-consistent perturbation calculation as described in Ref. 2. An external magnetic field which depends on both position and time is applied perpendicular to the magnetization, and the response of the system is determined. It is essential to take account of the rotation of the direction of magnetization,  $\hat{n}$ , in (2.1). Furthermore, if the external field has periodicity characterized by a wave-vector  $\vec{p}$ , the response of the system will involve a set of periodicities  $\vec{p} + \vec{K}_s$ , where  $\vec{K}_s$  is a reciprocal lattice vector. The result of these considerations is the formula for the wave-vector- and frequency-dependent transverse susceptibility matrix derived  $\chi_{+-}$  in Ref. 2. In matrix form (the matrix indices denote reciprocal-lattice vectors)

$$\chi = (1 - \chi_0 \Lambda)^{-1} \chi_0$$
 (2.4)

In this expression,  $\chi_0$  is the non-self-consistent susceptibility matrix, and we do not explicitly write the +- subscripts. We have

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$$[\chi_{0}(\vec{p},\omega)]_{ls} = -\frac{(g\mu_{B})^{2}}{N\Omega} \sum_{lnk} \frac{N_{n}(\vec{k}) - N_{l}(\vec{k} + \vec{p})}{E_{n}(\vec{k}) - E_{l}(\vec{k} + \vec{p}) + \omega + i\eta} \times \langle n\vec{k} | e^{-i\vec{p}_{l}\cdot\vec{r}}s_{+} | l\vec{k} + \vec{p} \rangle \langle l\vec{k} + \vec{p} | e^{i\vec{p}_{s}\cdot\vec{r}'}s_{-} | n\vec{k} \rangle .$$
(2.5)

The following conventions and notations apply:  $|\vec{nk}\rangle$  is a Bloch state belonging to band *n* and wave vector  $\vec{k}$ , its energy is  $E_n(\vec{k})$ , and its occupation number is  $N_n(\vec{k})$ . Since we are working at T=0 K in this paper,  $N_n(\vec{k})$  is either 1 or 0 according to the relation between  $E_n(\vec{k})$  and the Fermi energy. The operators  $s_+, s_-$  raise (or lower) the electron spin, while the quantity  $p_s$  is

$$\vec{\mathbf{p}}_s = \vec{\mathbf{p}} + \vec{\mathbf{K}}_s \; ,$$

g is the electron g factor  $\sim 2$ , and  $\mu_B$  is the Bohr magneton.

The other important object in Eq. (2.4) is  $\Lambda$ . This quantity is a matrix representation of  $V_f(\vec{r})/[g\mu_B M_0(\vec{r})]$  on a plane-wave basis,  $M_0(\vec{r})$  being the ground-state magnetization density. Specifically,

$$\Lambda_{ts} = \frac{1}{g\mu_B\Omega} \int_{\Omega} e^{i(\vec{K}_s - \vec{K}_l) \cdot \vec{r}} \frac{V_f(\vec{r})}{M_0(\vec{r})} d^3r \quad (2.6)$$

The integral includes a single unit cell of volume  $\Omega$ . It is convenient to regard  $\Lambda$  as a matrix product

$$\Lambda_{ts} = \frac{1}{g\mu_B} \sum_{u} (V_f)_{tu} (M_0^{-1})_{us} , \qquad (2.7)$$

where  $(V_f)_{su}$  is given by an expression similar to Eq. (2.6), etc. In the case of a crystal with inversion symmetry it is straightforward to show that the order of the factors  $V_f$  and  $M_0$ , is irrelevant. The spin-wave spectrum is determined by the poles of  $\chi$ , or equivalently, from the equation

$$\det(I - \chi_0 \Lambda) = 0 . \tag{2.8}$$

Since the quantities in Eq. (2.8) are matrices, this equation may lead to optical spin-wave modes.

It follows from very general considerations that there must be a spin-wave mode of energy  $\omega = 0$ when p=0. This is not an immediately obvious property of Eq. (2.8), but it is possible to transform this equation to a form in which the required property is apparent. A subsequent calculation also leads to an explicit expression for the spin-wave stiffness.

To do this, we note that Eq. (2.8) can be rewritten in the form

$$\det(g\mu_B M_0 - \chi_0 V_f) [\det(M_0)]^{-1} = 0 ,$$

or since  $det(M_0)$  should be nonsingular, it is sufficient to consider the equation

$$\det(g\mu_B M_0 - \chi_0 V_f) = 0.$$
 (2.9)

Let us consider the matix representing  $(\chi_0 V_f)$ . We multiply (2.5) by

$$V_f(\vec{\mathbf{K}}_s - \vec{\mathbf{K}}_u) = \Omega^{-1} \int_{\Omega}^{-i(\vec{\mathbf{K}}_s - \vec{\mathbf{K}}_u) \cdot \vec{\mathbf{r}}''} V_f^{(A)}(\vec{\mathbf{r}}'') d^3 r'',$$

(the superscript A indicates the contribution from a single cell), and sum over  $\vec{K}_s$  using the identity

$$\frac{1}{\Omega} \sum_{s} e^{i \vec{K}_{s} \cdot (\vec{r}' - \vec{r}'')} = \sum_{\mu} \delta(\vec{r}' - \vec{r}'' - \vec{R}_{\mu}) , \qquad (2.10)$$

in which  $\dot{R}_{\mu}$  is a direct lattice vector. We find

$$(\chi_0 V_f)_{tu} = -\frac{(g\mu_B)^2}{N\Omega} \sum_{lnk} \frac{N_n(\vec{k}) - N_l(\vec{k} + \vec{p})}{E_n(\vec{k}) - E_l(\vec{k} + \vec{p}) + \omega + i\eta} \times \langle n\vec{k} | e^{i\vec{p}_i \cdot \vec{r}} s_+ | l\vec{k} + \vec{p} \rangle \langle l\vec{k} + \vec{p} | s_- V_f e^{i(\vec{p} + \vec{k}_u) \cdot \vec{r}'} | n\vec{k} \rangle .$$
(2.11)

If we take the direction of the magnetization in the ground state to define the z axis, we then have

$$[H, s_{\pm}] = \pm V_f s_{\pm} .$$
 (2.12)

This relation enables us to rewrite the right-hand matrix element in (11) as

$$\langle l\vec{\mathbf{k}} + \vec{\mathbf{p}} | s_{-}V_{f}e^{i\vec{\mathbf{p}}_{u}\cdot\vec{\mathbf{r}}} | n\vec{\mathbf{k}} \rangle$$

$$= -\frac{1}{2} \{ [E_{l}(\vec{\mathbf{k}} + \vec{\mathbf{p}}) - E_{n}(\vec{\mathbf{k}})] \langle l\vec{\mathbf{k}} + \vec{\mathbf{p}} | e^{i\vec{\mathbf{p}}_{u}\cdot\vec{\mathbf{r}}} s_{-} | n\vec{\mathbf{k}} \rangle \langle \vec{\mathbf{k}} + \vec{\mathbf{p}} | e^{i\vec{\mathbf{p}}_{u}\cdot\vec{\mathbf{r}}} s_{-}(2i\vec{\mathbf{p}}_{u}\cdot\vec{\nabla} - \vec{\mathbf{p}}_{u}^{2}) | n\vec{\mathbf{k}} \rangle \} .$$

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From this, it follows that

$$(\chi_{0}V_{f})_{tu} = -\frac{(g\mu_{B})^{2}}{2N\Omega} \sum_{lnk} \left[ [N_{n}(\vec{k}) - N_{l}(\vec{k} + \vec{p})] \langle n\vec{k} | e^{-i\vec{p}_{t} \cdot \vec{n}} s_{+} | l\vec{k} + \vec{p} \rangle \right] \\ \times \left[ \langle l\vec{k} + \vec{p} | e^{i\vec{p}_{u} \cdot \vec{r}} s_{-} | n\vec{k} \rangle + \frac{\langle l\vec{k} + \vec{p} | e^{i\vec{p}_{u} \cdot \vec{r}} s_{-} (\vec{p}_{u}^{2} - 2i\vec{p}_{u} \cdot \vec{\nabla} - \omega) | n\vec{k} \rangle}{E_{n}(\vec{k}) - E_{l}(\vec{k} + \vec{p}) + \omega + i\eta} \right] \right].$$

$$(2.13)$$

This formula may be simplified through the use of closure and the properties of spin operators as follows:  $\sum_{l=k} [N_n(\vec{k}) - N_l(\vec{k} + \vec{p})] \langle n\vec{k} | e^{-i\vec{p}_l \cdot \vec{r}} s_+ | l\vec{k} + \vec{p} \rangle \langle l\vec{k} + \vec{p} | e^{i\vec{p}_u \cdot \vec{r}} s_- | n\vec{k} \rangle$ 

$$= 2 \sum_{nk} N_n(\vec{k}) \langle n \vec{k} | e^{-i(\vec{K}_t - \vec{K}_u) \cdot \vec{r}} s_z | n \vec{k} \rangle .$$

However, the magnetization density matrix is given through

.

$$M_{tu}^{(0)} \equiv M^{(0)}(\vec{K}_t - \vec{K}_u) = \frac{1}{N\Omega} (-g\mu_B) \sum_{nk} \langle n \vec{k} | e^{-i(\vec{K}_t - \vec{K}_u) \cdot \vec{r}} s_z | n \vec{k} \rangle .$$
(2.14)

Thus, finally,

$$(\chi_0 V_f)_{tu} = g\mu_B M_{tu}^{(0)} - \Delta_{tu} , \qquad (2.15a)$$

in which

$$\Delta_{tu} = \frac{1}{2} (\omega - p_u^2) [\chi_0(\vec{p}, \omega)]_{tu} - F_{tu}(\vec{p}, \omega)$$
(2.15b)

and

$$F_{tu}(\vec{p},\omega) = \frac{(g\mu_B)^2}{2N\Omega} \sum_{nlk} \frac{[N_n(\vec{k}) - N_l(\vec{k} + \vec{p})]}{E_n(\vec{k}) - E_l(\vec{k} + \vec{p}) + \omega + i\eta} \times \langle n\vec{k} | e^{-i\vec{p}_i \cdot \vec{r}} s_+ | l\vec{k} + \vec{p} \rangle \langle l\vec{k} + \vec{p} | e^{i\vec{p}_u \cdot \vec{r}} s_- (2i\vec{p}_u \cdot \vec{\nabla}) | n\vec{k} \rangle .$$
(2.15c)

Thus the determinantal Eq. (2.9) becomes

$$det[\Delta(p,\omega)] = 0. \qquad (2.16)$$

Note that if p=0 and  $\omega=0$ , the column of the matrix D corresponding to the zero reciprocallattice vector vanishes. In consequence, (2.16) is automatically satisfied under these circumstances, and there is necessarily a zero-energy spin-wave mode; the spin-wave spectrum is gapless. We can finally combine Eqs. (2.4), (2.7), and (2.15) to obtain a formula for the self-consistent susceptibility matrix, which we write in matrix notation as follows:

$$\chi = g\mu_B M_0 \Delta^{-1} \chi_0 . \qquad (2.17)$$

This expression for the susceptibility does not

contain explicit reference to the exchange-correlation potential. The quantities involved,  $M_0$ ,  $\Delta$ , and  $\chi_0$ , are determined from the energies and wave functions of the electron states. Of course, the exchange-correlation potential is explicitly involved in their determination. Equation (2.17) has the defect of requiring the evaluation of the inverse of an infinite matrix, which necessitates consideration of convergence problems. However, a problem of this sort is unavoidable if the possibility of investigation optical spin-wave models is of interest. Finally, we note that the element of  $\chi$  with  $K_s = K_t = 0$  in the static limit,  $\chi_{00}(p,0)$ , is for long wavelengths given by an expression which resembles that derived from a variational principle by Liu and Vosko.<sup>13</sup> However, no detailed equivalence has been derived.

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#### **III. THE SPIN-WAVE STIFFNESS**

For long-wavelength spin waves, we have

$$\omega = Dp^2 , \qquad (3.1)$$

where the constant D is known as the spin-wave stiffness. The general theory described above leads to a general expression for  $D^{11-13}$  The result obtained by Edwards and Rahman<sup>12</sup> is equivalent to

$$D = \frac{1}{n_{1} - n_{1}} \left[ n_{1} + n_{1} + \frac{1}{N} \sum_{ln \vec{k}} \frac{N_{n}(\vec{k}) - N_{l}(\vec{k})}{E_{n}(\vec{k}) - E_{l}(\vec{k})} \times \langle n\vec{k} | (\delta V - 2i\hat{p} \cdot \vec{\nabla})s_{+} | l\vec{k} \rangle \langle l\vec{k} | (2i\hat{p} \cdot \vec{\nabla})s_{-} | n\vec{k} \rangle \right].$$

$$(3.2)$$

Here,  $n_{\uparrow}$   $(n_{\downarrow})$  are the numbers of  $\uparrow$   $(\downarrow)$  spin electrons per cell, and  $\hat{p}$  is a unit vector in the direction of the spin-wave vector. The sum over  $\vec{k}$  effectively averages this over directions of  $\hat{p}$ . The quantity  $\delta V$  is the first-order (in p) change in the exchange-correlation potential produced by the presence of a magnetic disturbance of wave-vector p in the system:

$$\delta V = V_f(\vec{r}) \frac{1}{p} (m_p - 1)$$
, (3.3)

where  $m_p$  is the change in the magnetization density, which can be obtained from a self-consistency condition.<sup>12</sup> Equation (3.2) can be derived according to the procedures used here by introducing the Ansatz

$$\sum \left[ V_f(\vec{\mathbf{K}}_s) + \delta V_f(\vec{\mathbf{p}}, \vec{\mathbf{K}}_s) \right] \Delta_{s0} = 0 , \qquad (3.4)$$

in which  $\delta V_f(\vec{p},\vec{K}_s)$  is a Fourier coefficient of  $\delta V$  defined in Eq. (3.3). The argument is, in detail, sufficiently close to that given by Edwards and Rahman so that it will not be repeated here.

The quantity  $\delta V$  is rather complicated to evaluate, and actual computations so far have neglected this quantity. We believe that better calculations of *D* could be made based on the direct evaluation of the determinant  $\Delta$  in (2.16), a procedure which would allow study of the lifetimes as well as the energies of spin waves. However, our present results are for *D* only.

If  $\delta V$  is neglected and the system is assumed to have cubic symmetry, the equation for D simplifies to

$$D = \frac{1}{n_{\uparrow} - n_{\downarrow}} \left[ (n_{\uparrow} + n_{\downarrow}) + \frac{1}{3N} \sum_{lnk} \frac{N_{n}(\vec{k}) - N_{l}(\vec{k} + \vec{p})}{E_{n}(\vec{k}) - E_{l}(\vec{k})} |\langle n\vec{k} | s_{+}(-2i\nabla) | l\vec{k} \rangle |^{2} \right].$$
(3.5)

This form is not particularly convenient for numerical calculations because it gives D as the small difference between large numbers. It can, however, be transformed with the aid of the so-called f sum rule, which we can write (again assuming cubic symmetry) as

$$n_{1} + n_{\downarrow} = \frac{1}{3} \left[ \frac{1}{2} \sum_{n\vec{k}} N_{n}(\vec{k}) \nabla^{2} E_{n}(\vec{k}) - 4 \sum_{l(l \neq n)} \frac{|\langle n\vec{k} \mid \vec{p} \mid l\vec{k} \rangle|^{2}}{E_{n}(\vec{k}) - E_{l}(\vec{k})} N_{n}(\vec{k}) \right],$$
(3.6)

in which  $p = -i\nabla$  is now the momentum operator. Equation (3.5) can then be transformed into the expression

$$D = \frac{1}{6(n_{\uparrow} - n_{\downarrow})N} \left\{ \sum_{nk} N_{n}(\vec{k}) \nabla^{2} E_{n}(\vec{k}) + 8 \sum_{lnk} |\langle n\vec{k} | \vec{p}s_{+} | l\vec{k} \rangle |^{2} \frac{N_{n}(\vec{k}) - N_{l}(\vec{k})}{E_{n}(\vec{k}) - E_{l}(\vec{k})} - 8 \sum_{lnk} |\langle n\vec{k} | \vec{p} | l\vec{k} \rangle |^{2} \frac{N_{n}(\vec{k})[1 - N_{l}(\vec{k})]}{E_{n}(\vec{k}) - E_{l}(\vec{k})} \right\}.$$
(3.7)

This expression was evaluated for nickel using energy levels and wave functions obtained from an energy band calculation<sup>9</sup> based on the von Barth—Hedin (vBH) exchange potential.<sup>14</sup> A set of independent Gaussian orbitals (13s, 10p, 5d, 1f) was used as the basis for the band calculation. The use of Gaussian functions facilitates computation of the momentum matrix elements required in (3.6), and the full k dependence of energies and matrix elements is included in our calculation. The evaluation of (3.7) involved 505 points in  $\frac{1}{48}$  th of the Brillouin zone [corresponding to dividing the (100) axis into 16 equal parts]. Our result is

D = 0.148

in atomic units  $(\mathbf{Ry} a_0^2)$ .

The experimental value of D has been the subject of some controversy, as there appears to be a considerable discrepancy<sup>15</sup> between values obtained from neutron scattering measurements,<sup>16</sup> spin-wave resonance,<sup>17</sup> and studies of the temperature dependence of magnetization.<sup>15</sup> We choose the value obtained by Mook, Lynn, and Nicklow<sup>16</sup> from analysis of the temperature dependence of inelastic neutron scattering D=555 meV Å<sup>2</sup> (0.146 atomic units) for comparison with our result. The agreement, perhaps surprisingly, is excellent. However, it should be noted that results obtained by the other techniques mentioned (typically  $D \sim 0.10-0.11$  atomic units) are substantially lower. In view of the fact that the underlying band calculation produces an exchange splitting which is most likely too large, one would have expected the calculated D also to be too large. The convergence of the calculation with increasing number of k in the Brillouin zone needs to be investigated, as does the effect of including  $\delta V$  according to (3.2).

There may be some interest in comparing the present result for D obtained using the vBH potential with a value based on the Kohn-Sham potential. We estimate the latter to be 0.270, larger by a factor of almost 2 than the vBH result. The surprisingly large change results from the fact the second term in Eq. (3.7) (which in spite of its appearance is actually negative) is quite sensitive to the exchange splitting at the top of the d band. The exchange splitting obtained with the vBH potential is smaller by a factor of approximately 0.72 than that found with the Kohn-Sham potential. This factor accounts for most of the difference between the values of D.

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