High-temperature dynamical magnetic spin susceptibility of d-band metals

1990 J. Phys.: Condens. Matter 2 2215

(http://iopscience.iop.org/0953-8984/2/9/011)

J. Phys.: Condens. Matter **2** (1990) 2215–2230. Printed in the UK

High-temperature dynamical magnetic spin susceptibility of d-band metals

J Singh
Department of Physics, Punjab Agricultural University, Ludhiana-141004 (Punjab), India

Received 30 May 1989

Abstract. A formalism for the temperature-dependent dynamical magnetic spin susceptibility of d-band metals is developed in the framework of the generalised non-local model potential approach. Using the Shaw–Harrison model wavefunction transformation the magnetic spin susceptibility is separated into two parts: one is caused by the non-nodal character of the model wavefunction (i.e. the free-electron contribution) and the other by the depletion hole associated with the ion core. The latter is responsible for the Bloch character of conduction electrons and includes the s–d hybridisation effects in the d-band metals. The depletion hole contribution is calculated by two different approaches: the first is exact depletion hole approach and the second the averaged depletion hole approach. The calculations are performed for the spin susceptibility of V metal. The values of the depletion hole contribution in both approaches are found to be nearly the same quantitatively as well as qualitatively and are about 46% of the free-electron value. The spin susceptibility decreases and the peaks are broadened with increase in the temperature. The calculated and the experimental values of bulk magnetic spin susceptibility show reasonably good agreement and emphasise the importance of the depletion hole contribution.

1. Introduction

The d-band metals constitute a majority of elements in the periodic table and are of particular interest because of the peculiar behaviour of the d electrons (Marshall 1967, Doughlass 1975, 1976, Horton and Maradudin 1981). A frequency- and wavevector-dependent response function plays the central role in the study of many electronic properties of metals such as specific heat, resistivity, Lorentz number, ferromagnetism and superconductivity (Marshall 1967, Doughlass 1975, 1976, Horton and Maradudin 1981, Fay and Appel 1980). Therefore, a great deal of attention has been focused on studying the dynamical magnetic susceptibility—both spin and orbital contributions—of metallic systems as this can be directly compared with neutron scattering experiments (Löwde and Windsor 1970, Hebborn and March 1970, Mook *et al* 1973, Mook and Tocchetti 1979, Lynn and Mook 1981). The various spin susceptibility calculations can be categorised into two groups: the first is the localised spin model in which electrons are assumed to be localised at each atom and the second is the itinerant-electron model in which the electrons are represented by Bloch waves. The suitability of each model depends upon the nature of the element under consideration. The large electronic specific heat and fractional number of Bohr magnetrons per atom suggest that the itinerant-electron model is advantageous for the d-band metals (Izuyama *et al* 1963).

0953-8984/90/092215 + 16 $03.50

Neutron scattering experiments of the dynamical spin susceptibility of the d-band metals (Löwde and Windsor 1970, Mook and Tocchetti 1979, Lynn and Mook 1981) also support the itinerant-electron model. Johnson (1980) has shown, from the analysis of experimental positron annihilation data, that in the d-band metals a fraction of the d electrons have an itinerant character and the rest have a localised character. In V, Nb, Ta, Sc, Y, Ti and Zr all the d electrons have an itinerant character (Johnson 1980) and the itinerant d electrons can readily exchange with the conduction electrons (Stearns 1973, 1978).

The formal quantum theory of dynamical spin susceptibility $\chi^0(\boldsymbol{q}, \omega, T)$ has already been formulated in the itinerant-electron model (Izuyama *et al* 1963, Hebborn and March 1970) but its evaluation for d-electron metals is characteristically difficult. Here $\boldsymbol{q}$, ω and T are the field wavevector, frequency and temperature, respectively. The temperature-independent spin susceptibility $\chi^0(\boldsymbol{q}, \omega) = \chi^0(\boldsymbol{q}, \omega, 0)$ for the d electrons has been calculated by many workers (Löwde and Windsor 1970, Hebborn and March 1970, Diamond 1972, Liu 1976, Pickett and Allen 1977, Singh and Prakash 1977, Singh *et al* 1977, 1980, Sokoloff 1978, Stenzil and Winter 1985, 1986). A number of researchers (Doniach and Engelberg 1966, Shimizu *et al* 1962, Rivier and Zuckermann 1968) have emphasised the importance of the temperature dependence of $\chi^0(\boldsymbol{q}, \omega, T)$. The first attempt to incorporate this improvement was made by Kaiser and Doniach (1970) who gave a low-temperature expansion of $\chi^0(\boldsymbol{q}, \omega, T)$. Subsequently a few attempts have been made to calculate $\chi^0(\boldsymbol{q}, \omega, T)$ for paramagnetic substances (Jullien *et al* 1973, 1974, Singh *et al* 1981) but these calculations do not properly include the Bloch character of the electrons. In this paper, we formulate a model potential theory for the temperature dependence of the dynamical magnetic spin susceptibility of paramagnetic d-band metals in the itinerant-electron model which takes care of the Bloch character of the conduction electrons. The plan of the paper is as follows. In section 2, we give the necessary theory for the temperature-dependent magnetic spin susceptibility of the d-band metals. The formalism is applied to calculate the magnetic susceptibility of paramagnetic V. The results are presented and discussed in section 3. Finally, conclusions are drawn in section 4.

2. Theory

The general expression for the dynamical magnetic spin susceptibility of a paramagnetic metal in the random-phase approximation (RPA) is given by the well known expression (Hebborn and March 1970)

$$\chi^0(\boldsymbol{q}, \omega, T) = \tfrac{1}{2} g^2 \mu_B^2 \lim_{\varepsilon \to 0} \sum_{\boldsymbol{k}} L(\boldsymbol{k}, \boldsymbol{q}, \omega, T) M(\boldsymbol{k}, \boldsymbol{q}) \tag{1}$$

where

$$L(\boldsymbol{k}, \boldsymbol{q}, \omega, T) = [f(E_k, T) - f(E_{k+q}, T)]/[E_{k+q} - E_k - \hbar\omega - i\varepsilon] \tag{2}$$

and

$$M(\boldsymbol{k}, \boldsymbol{q}) = |\langle \psi_k(\boldsymbol{r}) | \exp(-i\boldsymbol{q} \cdot \boldsymbol{r}) | \psi_{k+q}(\boldsymbol{r}) \rangle|^2. \tag{3}$$

E_k is the energy eigenvalue corresponding to the Bloch state $\psi_k(\boldsymbol{r})$ with wavevector $\boldsymbol{k}$. μ_B is the Bohr magnetron, g is Lande's splitting factor and ε is a positive infinitesimal corresponding to the adiabatic switching on of a perturbing magnetic field. The function

$L(\boldsymbol{k}, \boldsymbol{q}, \omega, T)$ describes the band-structure effects and $M(\boldsymbol{k}, \boldsymbol{q})$ gives the effect of overlap matrix elements. The summation in equation (1) is over all occupied electronic states $\boldsymbol{k}$. $f(E_k, T)$ is the Fermi–Dirac distribution function given as

$$f(E_k, T) = [\![1 + \exp\{[E_k - E_F(T)]/k_B T\}]\!]^{-1}. \tag{4}$$

Here k_B is the Boltzmann constant and $E_F(T)$ is the temperature-dependent chemical potential which can be determined by the conservation of the number N of electrons in the conduction band as

$$2\sum_k f(E_k, T) = N. \tag{5}$$

The factor of 2 takes into account the spin degeneracy in a paramagnetic metal. The chemical potential at absolute zero is equal to the Fermi energy E_F, i.e. $E_F(0) = E_F = k_B T_F$, where T_F is the Fermi temperature. From now on we use the units $m = \hbar = k_B = 1$, where m is the free-electron mass. We shall solve equation (1) for $\chi^0(\boldsymbol{q}, \omega, T)$ by two approaches (the exact depletion hole (EDH) approach and the averaged depletion hole (ADH) approach) using the non-local model potential theory.

2.1. Exact depletion hole approach

Equation (1) for $\chi^0(\boldsymbol{q}, \omega, T)$ involves the true energy bands and the corresponding Bloch states and these can be determined from the one-electron Bloch wave equation

$$[-(1/2m^*)\nabla^2 + U(\boldsymbol{r})]\,|\psi_k(\boldsymbol{r})\rangle = E_k\,|\psi_k(\boldsymbol{r})\rangle. \tag{6}$$

Here m^* is the effective mass of the electrons, which includes band effects, and $U(\boldsymbol{r})$ is the crystal potential. The true Bloch wave equation can be transformed into a model wave equation

$$[-(1/2m^*)\nabla^2 + V_M(E, \boldsymbol{r})]\,|\varphi_k(\boldsymbol{r})\rangle = E_k\,|\varphi_k(\boldsymbol{r})\rangle \tag{7}$$

where $|\varphi_k(\boldsymbol{r})\rangle$ is the model wavefunction and $V_M(E, \boldsymbol{r})$ is the non-local (energy-dependent) model potential and is sufficiently general to include the model potential of Heine and Abarenkov (1964) (Animalu 1973) and the transition-metal pseudopotential of Harrison (1969). In the non-local model potential theory, Shaw and Harrison (1967) gave a model wavefunction transformation defined as

$$|\psi_k(\boldsymbol{r})\rangle = (1 - \partial V_M/\partial E)\,|\varphi_k(\boldsymbol{r})\rangle \tag{8}$$

where the energy derivative $\partial V_M/\partial E$ of the model potential has the properties of a projection operator, i.e.

$$(\partial V_M/\partial E)^2 = \partial V_M/\partial E. \tag{9}$$

In the d-band metals, equation (8) holds provided that the pole in V_M at $E = E_d$ (d-band energy) is handled appropriately by replacing $(E_d - E)^{-1}$ by $(E_d - E + i\frac{1}{2}W_d)^{-1}$ where W_d is the d-band width. For simplicity, $|\varphi_k(\boldsymbol{r})\rangle$ can be taken to be a plane wave defined as

$$|\varphi_k(\boldsymbol{r})\rangle = \Omega^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) = |\boldsymbol{k}\rangle \tag{10}$$

where Ω is the crystal volume. Using equations (8)–(10) and the properties of Bloch waves in the Wigner–Seitz approximation, one gets

$$\langle\psi_k(\boldsymbol{r})|\exp(-i\boldsymbol{q}\cdot\boldsymbol{r})\,|\psi_{k+q}(\boldsymbol{r})\rangle = 1 - \langle\boldsymbol{k}+\boldsymbol{q}|\partial V_M/\partial E|\boldsymbol{k}+\boldsymbol{q}\rangle. \tag{11}$$

Substituting equation (11) in equation (1), we get

$$\chi^0(\boldsymbol{q}, \omega, T) = \chi^0_{\mathrm{f}}(\boldsymbol{q}, \omega, T) + \chi^0_{\mathrm{dp}}(\boldsymbol{q}, \omega, T) \tag{12}$$

where

$$\chi^0_{\mathrm{f}}(\boldsymbol{q}, \omega, T) = \tfrac{1}{2}g^2\mu_{\mathrm{B}}^2 \lim_{\varepsilon\to 0}\left(\sum_{\boldsymbol{k}} L(\boldsymbol{k}, \boldsymbol{q}, \omega, T)\right) \tag{13}$$

$$\chi^0_{\mathrm{dp}}(\boldsymbol{q}, \omega, T) = \tfrac{1}{2}g^2\mu_{\mathrm{B}}^2 \lim_{\varepsilon\to 0}\left(\sum_{\boldsymbol{k}} L(\boldsymbol{k}, \boldsymbol{q}, \omega, T)\gamma(\boldsymbol{k}+\boldsymbol{q})\right) \tag{14}$$

$$\gamma(\boldsymbol{k}+\boldsymbol{q}) = \beta(\boldsymbol{k}+\boldsymbol{q}) + \tfrac{1}{4}|\beta(\boldsymbol{k}+\boldsymbol{q})|^2 \tag{15}$$

and

$$\beta(\boldsymbol{k}+\boldsymbol{q}) = \langle \boldsymbol{k}+\boldsymbol{q}| - 2(\partial V_{\mathrm{M}}/\partial E)|\boldsymbol{k}+\boldsymbol{q}\rangle. \tag{16}$$

$\chi^0_{\mathrm{f}}(\boldsymbol{q}, \omega, T)$ is the free-electron part of the magnetic spin susceptibility and is exactly the same expression as obtained by Hebborn and March (1970) and $\chi^0_{\mathrm{dp}}(\boldsymbol{q}, \omega, T)$ is the depletion hole contribution. $\gamma(\boldsymbol{k}+\boldsymbol{q})$ is called a depletion hole and is analogous to an orthogonalisation hole in the orthogonalised plane-wave theory. It should be noted that $\gamma(\boldsymbol{k}+\boldsymbol{q})$ gives the effect of overlap matrix elements and is a function of both $\boldsymbol{k}$ and $\boldsymbol{q}$. Using the Heine–Abarenkov model potential for the d-band metals the function $\beta(\boldsymbol{k}+\boldsymbol{q})$ has been calculated by us (Singh and Prakash 1981) and is given as

$$\beta(\boldsymbol{k}+\boldsymbol{q}) = \sum_{l=0}^{2} \beta_l(\boldsymbol{k}+\boldsymbol{q}) \tag{17}$$

where

$$\beta_l(\boldsymbol{k}+\boldsymbol{q}) = \frac{8\pi}{\Omega}(2l+1)\frac{\mathrm{d}A_l}{\mathrm{d}E}\int_0^{R_{\mathrm{M}}} [j_l(|\boldsymbol{k}+\boldsymbol{q}|r)]^2 r^2\,\mathrm{d}r. \tag{18}$$

R_{M} is the model radius and $j_l(|\boldsymbol{k}+\boldsymbol{q}|r)$ is a spherical Bessel function of order l. $\mathrm{d}A_l/\mathrm{d}E$ are energy derivatives of potential well depths $A_l(E)$ for $l = 0$, 1 and 2. $\mathrm{d}A_l/\mathrm{d}E$ for $l =$ 0 and 1 are calculated in the same way as by Singh and Prakash (1981) and $\mathrm{d}A_2/\mathrm{d}E$ is given as

$$\mathrm{d}A_2/\mathrm{d}E = A_2(E_{\mathrm{F}})(E_{\mathrm{F}} - E_{\mathrm{d}})/[(E_{\mathrm{d}} - E)^2 + (\tfrac{1}{2}W_{\mathrm{d}})^2]. \tag{19}$$

The singularity at $E = E_{\mathrm{d}}$ is handled by using the **t**-matrix method. From equations (17) and (18) it is evident that $\beta(\boldsymbol{k}+\boldsymbol{q})$ and therefore $\gamma(\boldsymbol{k}+\boldsymbol{q})$ have a finite value at $|\boldsymbol{q}| = 0$. In the parabolic band approximation the limiting value of $\chi^0(\boldsymbol{q}, \omega, T)$ can be calculated. It can straightaway be proved that, at $|\boldsymbol{q}| = \omega = T = 0$,

$$\chi^0_{\mathrm{f}}(0,0,0) = \chi^{\mathrm{P}}_{\mathrm{f}} = \tfrac{1}{2}g^2\mu_{\mathrm{B}}^2 N_{\mathrm{f}}(E_{\mathrm{F}}) = \tfrac{1}{2}g^2\mu_{\mathrm{B}}^2(m^* k_{\mathrm{F}}\Omega/2\pi^2) \tag{20}$$

$$\chi^0_{\mathrm{dp}}(0,0,0) = \gamma_0\chi^{\mathrm{P}}_{\mathrm{f}} \tag{21}$$

where $\chi^{\mathrm{P}}_{\mathrm{f}}$ is the Pauli spin susceptibility for free electrons and $N_{\mathrm{f}}(E_{\mathrm{F}})$ is the free-electron density of states (DOS) at E_{F} for single spin. Here γ_0 is the value of $\gamma(\boldsymbol{k}+\boldsymbol{q})$ at $|\boldsymbol{q}| = 0$ obtained by summing over all $\boldsymbol{k}$-values in equation (14). The total Pauli spin susceptibility for a metallic system becomes

$$\chi^{\mathrm{P}} = (1+\gamma_0)\chi^{\mathrm{P}}_{\mathrm{f}}. \tag{22}$$

To compare the free-electron and depletion hole contributions to the spin susceptibility, we define the reduced susceptibility as

$$\overline{\chi^0}(q, \omega, T) = \chi^0(q, \omega, T)/\chi^0_f(0, 0, 0)$$
$$= \overline{\chi^0_f}(q, \omega, T) + \overline{\chi^0_{dp}}(q, \omega, T). \tag{23}$$

In this way, $\overline{\chi^0_f}(q, \omega, T)$ is normalised to unity at $|q| = \omega = T = 0$. Therefore the relative magnitude of $\overline{\chi^0_{dp}}(q, \omega, T)$ with respect to $\overline{\chi^0_f}(q, \omega, T)$ can be readily found. The real and imaginary parts of $\chi^0(q, \omega, T)$ can be separated using the identity

$$\lim_{\varepsilon \to 0}[1/(x \pm i\varepsilon)] = 1/x \mp i\pi\delta(x). \tag{24}$$

Therefore the imaginary part of $\overline{\chi^0_f}(q, \omega, T)$ from equations (13), (23) and (24) can be written as

$$\operatorname{Im} \overline{\chi^0_f}(q, \omega, T) = \frac{2\pi^3}{m^* k_F \Omega} \sum_k [f(E_k, T) - f(E_{k+q}, T)]\delta(E_{k+q} - E_k - \omega). \tag{25}$$

Transforming the summation into an integration and solving it analytically, one obtains

$$\operatorname{Im} \overline{\chi^0_f}(q, \omega, T) = (\pi/2)(T/qv_F) \ln[\{\exp(\omega/T)$$
$$+ \exp[\varepsilon(q, \omega, T)/T]\}/\{1 + \exp[\varepsilon(q, \omega, T)/T]\}] \tag{26}$$

where

$$\varepsilon(q, \omega, T) = (1/2m^*)|m^*\omega/|q| + |q|/2|^2 - E_F(T) \tag{27}$$

and $v_F = k_F/m^*$ is the Fermi velocity. In equation (14) for $\chi^0_{dp}(q, \omega, T)$ the angular integral can be solved in the same manner as for $\chi^0_f(q, \omega, T)$ but the analytical integration over k is rendered incalculable because $\gamma(k + q)$ itself is in the integral form. The imaginary part of $\overline{\chi^0_{dp}}(q, \omega, T)$ becomes

$$\operatorname{Im} \overline{\chi^0_{dp}}(q, \omega, T) = \frac{\pi}{2qk_F} \int_{|m^*\omega/q - q/2|}^{\infty} dk\, k[f(E_k, T) - f(E_k + \omega, T)]\gamma(k + q). \tag{28}$$

The imaginary part of the total susceptibility $\overline{\chi^0}(q, \omega, T)$ is the sum of two contributions given by equations (26) and (28), i.e.

$$\operatorname{Im} \overline{\chi^0}(q, \omega, T) = \operatorname{Im} \overline{\chi^0_f}(q, \omega, T) + \operatorname{Im} \overline{\chi^0_{dp}}(q, \omega, T). \tag{29}$$

The real part of $\overline{\chi^0}(q, \omega, T)$ can be calculated using the Kramer–Kronig relation

$$\operatorname{Re} \overline{\chi^0}(q, \omega, T) = \frac{2}{\pi} \int_0^{\infty} \frac{\omega' \operatorname{Im} \overline{\chi^0}(q, \omega', T)}{(\omega')^2 - \omega^2} d\omega'. \tag{30}$$

Substituting equation (29) in equation (30), we write

$$\operatorname{Re} \overline{\chi^0}(q, \omega, T) = \operatorname{Re} \overline{\chi^0_f}(q, \omega, T) + \operatorname{Re} \overline{\chi^0_{dp}}(q, \omega, T). \tag{31}$$

2.2. Averaged depletion hole approach

In the derivation of equation (28) the depletion hole $\gamma(k + q)$ is a function of both k and q. Shaw and Harrison (1967) defined ADH by summing over all the occupied electronic

states as

$$\gamma(\boldsymbol{q}, T) = \frac{1}{Z}\sum_{k} f(E_k, T)\gamma(\boldsymbol{k}+\boldsymbol{q}). \tag{32}$$

Z is the valency of the metallic system. The ADH $\gamma(\boldsymbol{q}, T)$ becomes temperature dependent via the Fermi distribution function. Using equation (15) in equation (32) and simplifying by changing the summation into integration, we get

$$\gamma(\boldsymbol{q}, T) = \beta(\boldsymbol{q}, T) + \xi(\boldsymbol{q}, T) \tag{33}$$

where

$$\beta(\boldsymbol{q}, T) = \frac{\Omega}{\pi^2 Z}\int_0^\infty \mathrm{d}k\, k^2 f(E_k, T)\beta(\boldsymbol{k}+\boldsymbol{q}) \tag{34}$$

$$\xi(\boldsymbol{q}, T) = \frac{\Omega}{\pi^2 Z}\int_0^\infty \mathrm{d}k\, k^2 f(E_k, T)[\tfrac{1}{4}|\beta(\boldsymbol{k}+\boldsymbol{q})|^2]. \tag{35}$$

$\beta(\boldsymbol{q}, T)$ and $\xi(\boldsymbol{q}, T)$ give the first- and second-order contributions, respectively, to $\gamma(\boldsymbol{q}, T)$. At absolute zero temperature we get the same expression for ADH as obtained by Singh and Prakash (1981).

Using $\gamma(\boldsymbol{q}, T)$ instead of $\gamma(\boldsymbol{k}+\boldsymbol{q})$ in equation (14) for $\chi^0_{\mathrm{dp}}(\boldsymbol{q}, \omega, T)$, we write

$$\chi^0_{\mathrm{dp}}(\boldsymbol{q}, \omega, T) = \tfrac{1}{2}g^2\mu_{\mathrm{B}}^2\gamma(\boldsymbol{q}, T)\lim_{\varepsilon\to 0}\left(\sum_{k} L(\boldsymbol{k}, \boldsymbol{q}, \omega, T)\right) = \gamma(\boldsymbol{q}, T)\chi^0_{\mathrm{f}}(\boldsymbol{q}, \omega, T). \tag{36}$$

Therefore in the ADH approximation the total spin susceptibility from equation (12) becomes

$$\chi^0(\boldsymbol{q}, \omega, T) = [1 + \gamma(\boldsymbol{q}, T)]\chi^0_{\mathrm{f}}(\boldsymbol{q}, \omega, T) \tag{37}$$

and, in the limit $|\boldsymbol{q}| = \omega = T = 0$, it reduces to the Pauli spin susceptibility χ^{P} given as

$$\chi^{\mathrm{P}} = [1 + \gamma(0, 0)]\chi^{\mathrm{P}}_{\mathrm{f}}. \tag{38}$$

The real and imaginary parts of $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ in the ADH approximation are given as

$$\begin{aligned} \mathrm{Im}\,\overline{\chi^0}(\boldsymbol{q}, \omega, T) &= [1 + \gamma(\boldsymbol{q}, T)]\,\mathrm{Im}\,\overline{\chi^0_{\mathrm{f}}}(\boldsymbol{q}, \omega, T) \\ \mathrm{Re}\,\overline{\chi^0}(\boldsymbol{q}, \omega, T) &= [1 + \gamma(\boldsymbol{q}, T)]\,\mathrm{Re}\,\overline{\chi^0_{\mathrm{f}}}(\boldsymbol{q}, \omega, T). \end{aligned} \tag{39}$$

$\mathrm{Re}\,\overline{\chi^0_{\mathrm{f}}}(\boldsymbol{q}, \omega, T)$ is obtained from $\mathrm{Im}\,\overline{\chi^0_{\mathrm{f}}}(\boldsymbol{q}, \omega, T)$ using the Kramer–Kronig relation.

Table 1. Model potential parameters for V metal in atomic units taken from Singh *et al* (1980); k_{d} is the wavevector for the d band of V metal.

Z	5.0
m^*	2.2
k_{F}	1.164
R_{M}	1.6
Ω_0 (atomic volume)	93.9
$A_2(E_{\mathrm{F}})$	2.9
k_{d}	0.64
W_{d}	0.24
$\mathrm{d}A_0/\mathrm{d}E$	0.0
$\mathrm{d}A_1/\mathrm{d}E$	1.56

It should be pointed out that, if a local model potential is used in place of the non-local potential, $\gamma(q, T)$, $\gamma(k+q)$ and hence $\chi^0_{dp}(q, \omega, T)$ reduce to zero and the conventional free-electron metal theory for $\chi^0(q, \omega, T)$ is retrieved (Hebborn and March 1970). Therefore, $\chi^0_{dp}(q, \omega, T)$ includes the non-local effects arising from the s, p and d characters of the conduction electrons. It takes into account the resonant character of the d electrons (see equation (19)) which is analogous to the s–d hybridisation of the orthogonalised plane-wave pseudopotential theory (Harrison 1969).

3. Results and discussion

The formalism is applied to calculate $\chi^0(q, \omega, T)$ for paramagnetic V metal where $\chi^0_{dp}(q, \omega, T)$ is expected to be large. The unique relation between $E_F(T)$ and T is obtained by solving numerically equation (5). The numerical calculation of $\chi^0(q, \omega, T)$ also requires knowledge of band-structure and model potential parameters. The effective mass m^* of the conduction electrons is estimated from the mass enhancement factor $\lambda = m^*/m - 1$, where λ is taken to be 1.22 from the muffin-tin calculations of MacDonald (1981) and Papaconstantopoulos *et al* (1977). The model potential and other physical parameters of V metal are given in table 1. Figures 1(*a*) and 1(*b*) show the ADH $\gamma(q, T)$ as a function of q and T for V metal. These show that $\gamma(q, T)$ decreases with increases in q and T. At large values of q, $\gamma(q, T)$ approaches approximately the same value at all temperatures. At small values of q, $\gamma(q, T)$ exhibits a small peak which is due to the resonant behaviour of $\beta_2(k+q)$ (see equations (18) and (19)). This peak is weakened with the increase of T and finally disappears. Further it is found that, on decreasing W_d, the magnitude and peak strength of $\beta_2(k+q)$ and hence of $\gamma(q, T)$ increase. Therefore in metals with narrow d bands (e.g. ferromagnetic metals) the d-band contribution forms the major part of $\gamma(q, T)$. In V metal at $q = T = 0$, the depletion hole $\gamma(0, 0) = 0.458$; therefore it enhances the spin magnetic susceptibility. The d-band contribution to $\gamma(0, 0)$ is 0.283 which dominates the s- and p-band contributions having a value 0.175.

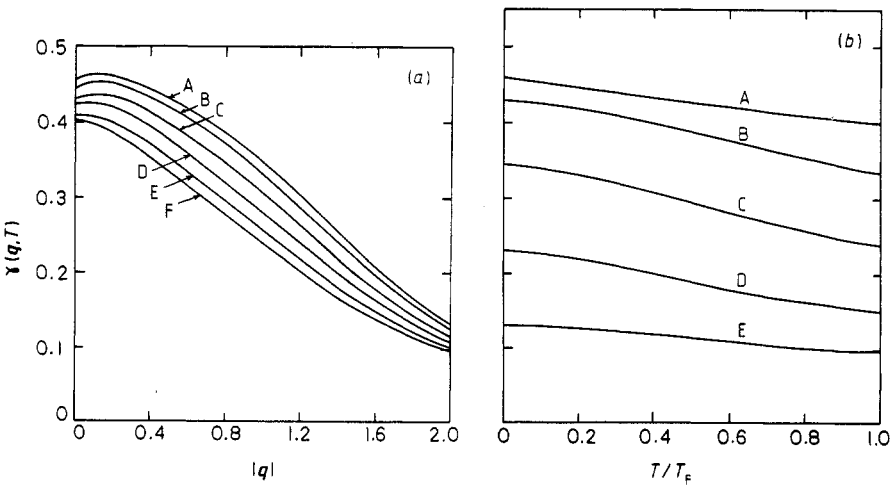

Figure 1. (*a*) Computed $\gamma(q, T)$ versus q for different T/T_F-values: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$; curve C, $T/T_F = 0.4$; curve D, $T/T_F = 0.6$; curve E, $T/T_F = 0.8$; curve F, $T/T_F = 1.0$. (*b*) $\gamma(q, T)$ as a function of T/T_F for different q-values ($W_d = 0.48$ Ryd): curve A, $|q| = 0$; curve B, $|q| = 0.5$; curve C, $|q| = 1.0$; curve D, $|q| = 1.5$; curve E, $|q| = 2.0$.

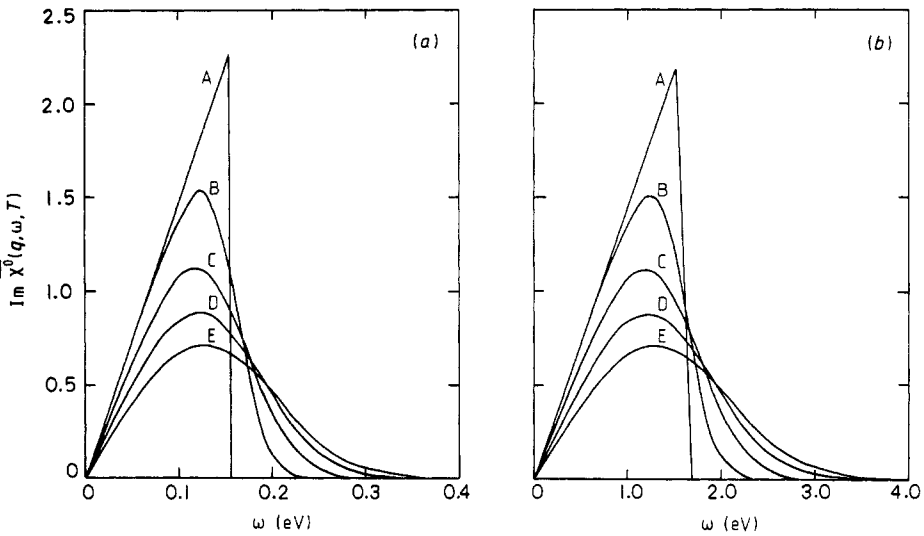

Figure 2. Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ versus ω, evaluated in the EDH approach, for (*a*) $|\boldsymbol{q}| = 0.005$ and (*b*) $|\boldsymbol{q}| = 0.05$ au: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$; curve C, $T/T_F = 0.4$; curve D, $T/T_F = 0.6$; curve E, $T/T_F = 0.8$.

$\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ is calculated for paramagnetic V using both the EDH and the ADH approaches. Figure 2 shows Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ as a function of ω for selected values of $\boldsymbol{q}$ and T in the EDH approach. In general, Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ collapses and the peak is broadened with increase in T. It should be noticed (figure 2) that, as the value of $|\boldsymbol{q}|$ is increased from 0.005 to 0.05 au, the range of ω also increases in the same order while the shape of the Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ curve remains nearly the same. Figure 3(*a*) shows $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ for three different values of W_d at $|\boldsymbol{q}| = 0.005$ au and $T/T_F = 0.2$. It is found that Im $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ changes only by a small amount near the peak position even with 20% change in W_d. Therefore in V metal the broadening of the peak and the decrease in magnitude of Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ is caused mainly by the Fermi distribution functions. Im $\overline{\chi^0_f}(\boldsymbol{q}, \omega, T)$ and Im $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ for $|\boldsymbol{q}| = 0.005$ au and $T/T_F = 0.2$, are shown separately in figure 3(*b*) to make a direct comparison between them. Both Im $\overline{\chi^0_f}(\boldsymbol{q}, \omega, T)$ and Im $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ exhibit a peak at the same energy $\omega = 0.15$ eV. $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ is finite over an appreciable energy range although less than that of $\overline{\chi^0_f}(\boldsymbol{q}, \omega, T)$. It is due to the inclusion of s–d hybridisation which increases the d-band width and hence makes the d electrons quasi-localised. Singh *et al* (1981) calculated $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ for the d-band metals in the tight-binding approximation, neglecting the s–d hybridisation, and found the d-band contribution to be strongly localised to a small energy region.

Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ has also been calculated in the ADH approximation and is shown in figure 4 for $|\boldsymbol{q}| = 0.005$ au and at various T-values. It is found that the values of Im $\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ are approximately the same in both the EDH and the ADH approaches. As only $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ differs in the two approaches, therefore a more apparent comparison can be made by comparing Im $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$. Figure 5 shows Im $\overline{\chi^0_{dp}}(\boldsymbol{q}, \omega, T)$ as a function of ω and it is found that the two approaches yield approximately the same values along the entire energy and temperature range. Therefore, the temperature-dependent ADH approach gives correct results for the magnetic spin susceptibility.

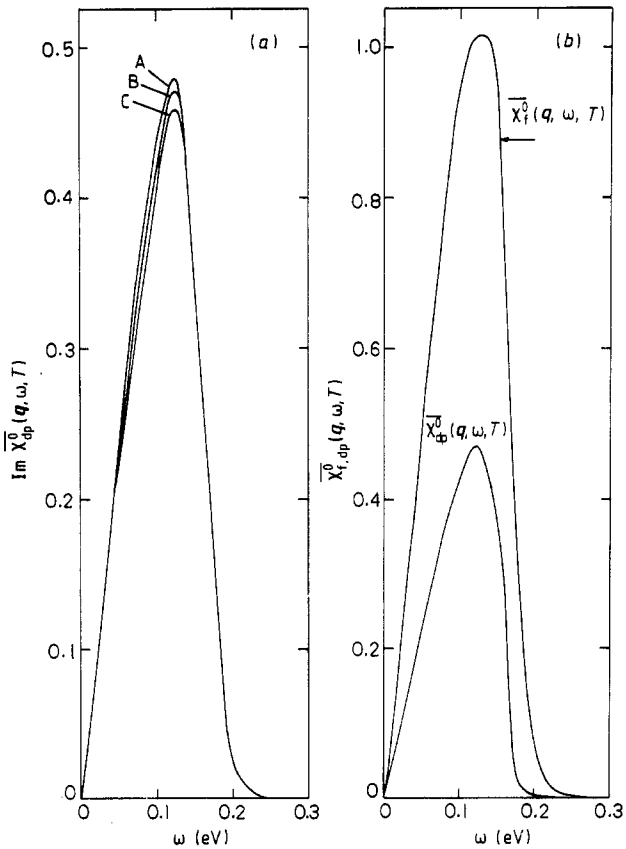

Figure 3. (*a*) Im $\overline{\chi^0_{dp}}(q, \omega, T)$, in the EDH approach, as a function of ω for (*a*) $|q| = 0.005$ au and $T/T_F = 0.2$: curve A, $\frac{1}{2}W_d = 0.19$ Ryd; curve B, $\frac{1}{2}W_d = 0.24$ Ryd; curve C, $\frac{1}{2}W_d = 0.29$ Ryd. (*b*) Im $\overline{\chi^0_f}(q, \omega, T)$ and Im $\overline{\chi^0_{dp}}(q, \omega, T)$, in the EDH approach, as a function of ω for $|q| = 0.005$ au and $T/T_F = 0.2$.

Re $\overline{\chi^0}(q, \omega, T)$ as a function of ω is shown in figure 6 in both the approaches. The results are shown only at two T-values at $|q| = 0.005$ au as the calculation of Re $\overline{\chi^0}(q, \omega, T)$ consumes much computer time. At particular q- and T-values, Re $\overline{\chi^0}(q, \omega, T)$ decreases rapidly with increasing ω, becoming negative with a minimum at $\omega = 0.157$ eV, and thereafter smoothly tends to zero with increasing ω-values. It should be noted that the minimum in Re $\overline{\chi^0}(q, \omega, T)$ occurs at the same energy at which the peak in Im $\overline{\chi^0}(q, \omega, T)$ is found (see figures 2 and 4). Both the approaches give approximately the same results for Re $\overline{\chi^0}(q, \omega, T)$. As no experimental results on $\overline{\chi^0}(q, \omega, T)$ for V metal are available, therefore the comparison of the results as such is not possible, but one can study the limiting cases of $\overline{\chi^0}(q, \omega, T)$ and compare the trend of the results with the available experimental and theoretical information.

Im $\overline{\chi^0}(q, \omega, T)$ given by equation (39) in the ADH approach reduces at absolute zero to

$$\text{Im}\,\overline{\chi^0}(q, \omega, T) = [1 + \gamma(q)]\,\text{Im}\,\overline{\chi^0_f}(q, \omega, T) \tag{40}$$

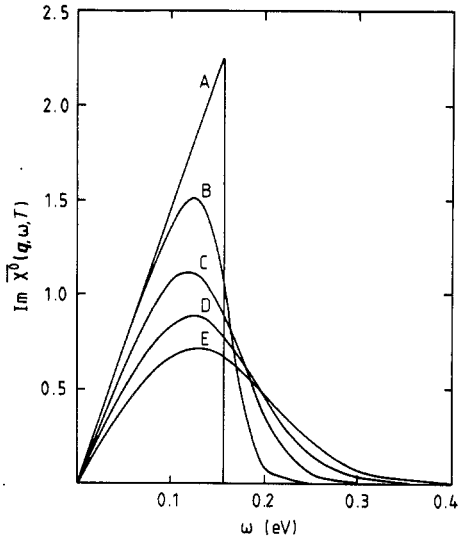

Figure 4. Im $\overline{\chi^0}(q, \omega, T)$, evaluated in the ADH approach, versus ω for $|q| = 0.005$ au: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$; curve C, $T/T_F = 0.4$; curve D, $T/T_F = 0.6$; curve E, $T/T_F = 0.8$.

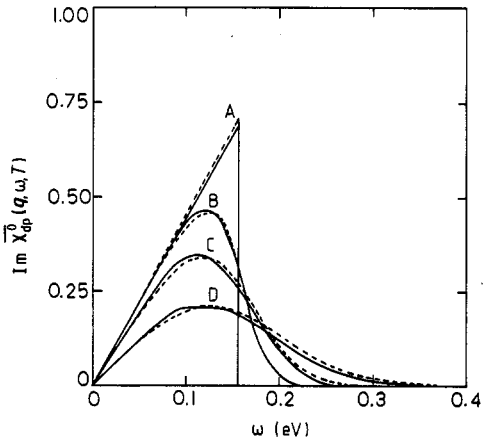

Figure 5. Im $\overline{\chi^0_{dp}}(q, \omega, T)$ versus ω and T for fixed $|q| = 0.005$ au evaluated in the EDH (——) and ADH (– – –) approaches: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$; curve C, $T/T_F = 0.4$; curve D, $T/T_F = 0.8$.

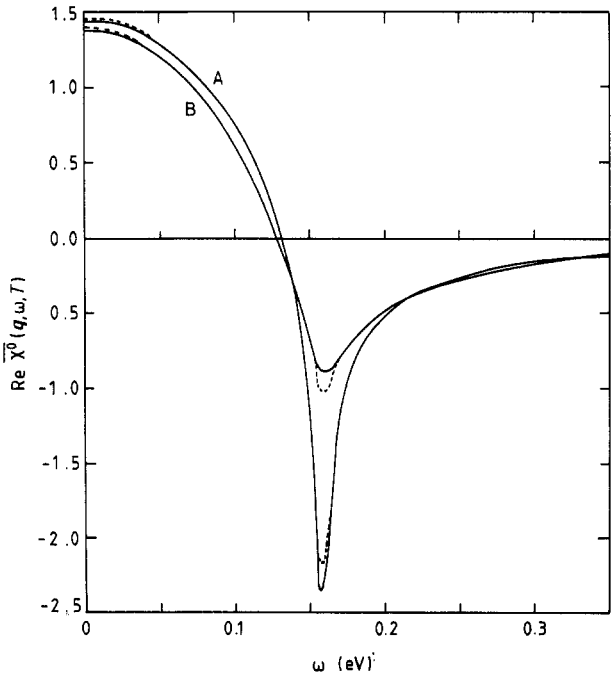

Figure 6. Re $\overline{\chi^0}(q, \omega, T)$ versus ω for $|q| = 0.005$ au evaluated in the ADH (——) and EDH (– – –) approaches: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$.

where

$$\operatorname{Im}\overline{\chi_f^0}(\boldsymbol{q}, \omega, T) = (\pi/8\lambda)\{[1 - (m^*W/\lambda - \lambda)^2]\theta[1 - (m^*W/\lambda - \lambda)^2] - [1 - (m^*W/\lambda + \lambda)^2]\theta[1 - (m^*W/\lambda + \lambda)^2]\} \tag{41}$$

and $\lambda = q/2k_F$, $W = \omega/2k_F^2$. Equation (39) for $\operatorname{Re}\overline{\chi^0}(\boldsymbol{q}, \omega, T)$ reduces, at absolute zero, to

$$\operatorname{Re}\overline{\chi^0}(\boldsymbol{q}, \omega, 0) = [1 + \gamma(\boldsymbol{q})]\operatorname{Re}\overline{\chi_f^0}(\boldsymbol{q}, \omega, 0) \tag{42}$$

where

$$\operatorname{Re}\overline{\chi_f^0}(\boldsymbol{q}, \omega, 0) = \tfrac{1}{2} + (1/8\lambda)[1 - (m^*W/\lambda - \lambda)^2] \times \ln|(1 - m^*W/\lambda + \lambda)/(1 + m^*W/\lambda - \lambda)| - (1/8\lambda) \times [1 - (m^*W/\lambda + \lambda)^2]\ln|(1 - m^*W/\lambda - \lambda)/(1 + m^*W/\lambda + \lambda)|. \tag{43}$$

Equations (41) and (43) are exactly the same expressions as obtained by Hebborn and March (1970) and define the classical Lindhard function for free-electron metals. In the EDH approach the expressions for $\operatorname{Re}\overline{\chi_f^0}(\boldsymbol{q}, \omega, 0)$ and $\operatorname{Im}\overline{\chi_f^0}(\boldsymbol{q}, \omega, 0)$ are the same as given above but it is not possible to get an analytical expression for $\overline{\chi_{dp}^0}(\boldsymbol{q}, \omega, 0)$. The results for $\operatorname{Im}\overline{\chi^0}(\boldsymbol{q}, \omega, 0)$, evaluated in the EDH and ADH approaches, are shown in figures 2 and 4 and are approximately the same. $\operatorname{Re}\overline{\chi^0}(\boldsymbol{q}, \omega, 0)$ in both approaches is shown in figure 6.

The temperature-dependent static spin susceptibility $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ is obtained from the Kramer–Kronig relation (30) by substituting $\omega = 0$ in it. In the ADH approach, $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ is given as

$$\overline{\chi^0}(\boldsymbol{q}, 0, T) = [1 + \gamma(\boldsymbol{q}, T)]\overline{\chi_f^0}(\boldsymbol{q}, 0, T) \tag{44}$$

and is a real quantity. It is not possible to obtain an analytical expression for $\overline{\chi_f^0}(\boldsymbol{q}, 0, T)$ but one can immediately obtain, for very high temperatures,

$$\overline{\chi^0}(\boldsymbol{q}, 0, T) = [1 + \gamma(\boldsymbol{q}, T)]\tfrac{2}{3}T_F/T. \tag{45}$$

If one neglects the depletion hole contribution, one obtains the usual Curie law for free-electron metals. Equation (45) therefore gives the Curie law for the d-band metals which show a departure from the usual Curie law. Shimizu (1981) pointed out that there is a deviation from the standard Curie law in all the paramagnetic and ferromagnetic substances due to spin fluctuations in an itinerant-electron model. At $T = 0$, equation (44) reduces to

$$\overline{\chi^0}(\boldsymbol{q}, 0, 0) = [1 + \gamma(\boldsymbol{q}, 0)]\overline{\chi_f^0}(\boldsymbol{q}, 0, 0) \tag{46}$$

with

$$\overline{\chi_f^0}(\boldsymbol{q}, 0, 0) = \tfrac{1}{2} + (1/4\lambda)(1 - \lambda^2)\ln|(1 + \lambda)/(1 - \lambda)|. \tag{47}$$

Equation (47) is the static Lindhard function for the free-electron gas and exhibits a Kohn anomaly (logarithmic singularity) at $q = 2k_F$. $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ calculated in the ADH approach, for the V metal is shown in figure 7. At $|\boldsymbol{q}| = T = 0$, $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ is equal to $1 + \gamma(0, 0) = 1.458$ while, in the EDH approach, $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ is equal to $1 + \gamma_0 = 1.467$ which is very close to the above value. Therefore, the depletion hole contributes towards the Pauli spin susceptibility by about 46% of χ_f^P. At $T = 0$ K, $\overline{\chi^0}(\boldsymbol{q}, 0, T)$ exhibits a Kohn anomaly at $q = 2k_F$ (see figure 7 and equation (46)) which is weakened with the

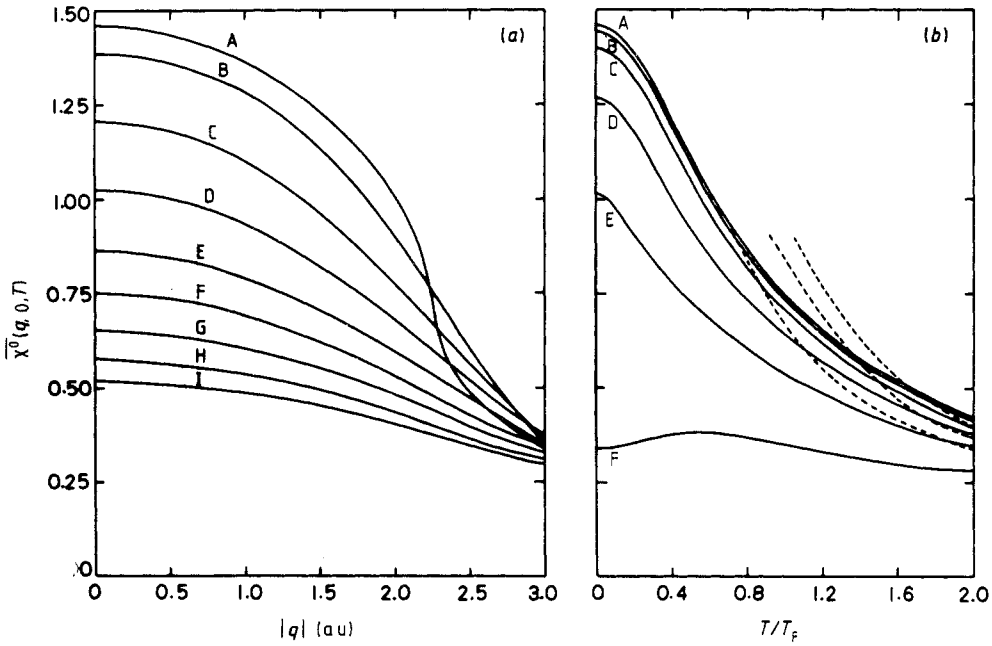

Figure 7. (*a*) $\overline{\chi^0}(q, 0, T)$, calculated in the ADH approach, versus $|q|$: curve A, $T/T_F = 0$; curve B, $T/T_F = 0.2$; curve C, $T/T_F = 0.4$; curve D, $T/T_F = 0.6$; curve E, $T/T_F = 0.8$; curve F, $T/T_F = 1.0$; curve G, $T/T_F = 1.2$; curve H, $T/T_F = 1.4$; curve I, $T/T_F = 1.6$. (*b*) $\chi^0(q, 0, T)$, calculated in the ADH approach, versus T/T_F; curve A, $|q| = 0.005$ au; curve B, $|q| = 0.4$ au curve C, $|q| = 0.8$ au; curve D, $|q| = 1.4$ au; curve E, $|q| = 2.0$ au; curve F, $|q| = 3.0$ au; – – –, modified Curie behaviour, in descending order, for $|q| = 0.005$, $|q| = 2.0$ and $|q|$ very large.

increase in T and finally it disappears owing to the smearing of the Fermi surface. In figure 7 is also shown the Curie behaviour, given by equation (45), for different q-values. Further in the present formalism the behaviours of $\overline{\chi^0_f}(q, 0, T)$ and $\overline{\chi^0_{dp}}(q, 0, T)$ are found to be similar. At small T-values (ranging from 0 to 300 K), $\overline{\chi^0}(0, 0, T)$ decreases approximately linearly with increasing T but the decrease is quite small as found experimentally (Kreissman and Callen 1954, Akoh and Tasaki 1977). However, at low temperatures the thermal expansion must be taken into account to get the correct T variation.

So far in the calculation of $\overline{\chi^0}(q, \omega, T)$ the electrons are treated as non-interacting particles but actually these interact with each other, giving rise to exchange and correlation effects. The quantitative calculations of magnetic susceptibility require the inclusion of the exchange and correlation effects which enhance the magnetic susceptibility. The exchange and correlation effects are difficult to deal with and therefore are incorporated in different approximations (Kohn and Sham 1965, Vosko and Perdew 1975, Janak 1977). In the RPA the exchange-enhanced magnetic spin susceptibility is given as (Hebborn and March 1970)

$$\chi(q, \omega, T) = \chi^0(q, \omega, T)/[1 - (2/g^2\mu_B^2)I(q, T)\chi^0(q, \omega, T)] \qquad (48)$$

where $I(q, T)$ is a q- and T-dependent phenomenological electron–electron interaction parameter. The exact dependence of $I(q, T)$ on q and T is not known; therefore, it is estimated in different limiting cases (Doniach 1967, Allan *et al* 1968, Singwi *et al* 1970,

Janak 1977). In view of these uncertainties, $I(q, T)$ is taken to be independent of q and T in the present investigations. The exchange-enhanced reduced spin susceptibility, therefore, becomes

$$\bar{\chi}(q, \omega, T) = \overline{\chi^0}(q, \omega, T)/[1 - \bar{I}\overline{\chi^0}(q, \omega, T)] \tag{49}$$

where $\bar{I} = IN_f(E_F)$. In the limit $q = \omega = T = 0$, equation (49) gives the effective Stoner enhancement factor S_{eff} as

$$S_{eff} = [1 + \gamma(0, 0)]/[1 - IN(E_F)] = S^* + S^*_{dp} \tag{50}$$

where

$$S^* = 1/[1 - IN(E_F)] \tag{51}$$

$$S^*_{dp} = \gamma(0, 0)/[1 - IN(E_F)] \tag{52}$$

$$N(E_F) = [1 + \gamma(0, 0)]N_f(E_F) \tag{53}$$

$N(E_F)$ is the total DOS at E_F. S^*_{dp} is the Stoner enhancement due to the depletion hole although S^* also includes the depletion hole contribution indirectly through $N(E_F)$. As the depletion hole contribution approaches zero, S_{eff} reduces to the usual Stoner enhancement factor due to the free electrons and is given as

$$S_f = 1/(1 - \bar{I}). \tag{54}$$

From equation (50) it is evident that $S_{eff} > S_f$ in the d-band metals with a positive depletion hole contribution, as in V metal, and $S_{eff} < S_f$ in other metals with a negative depletion hole contribution.

The exchange-enhanced static reduced spin susceptibility from equation (49) can be written as

$$\bar{\chi}(q, 0, T) = \overline{\chi^0}(q, 0, T)/[1 - \bar{I}\overline{\chi^0}(q, 0, T)]. \tag{55}$$

Figure 8 shows $\bar{\chi}(q, 0, T)$ for V metal, as a function of T for $S_{eff} = 10$ (hypothetical value). $\bar{\chi}(q, 0, T)$ starts with a value equal to S_{eff} and decreases very rapidly with increase

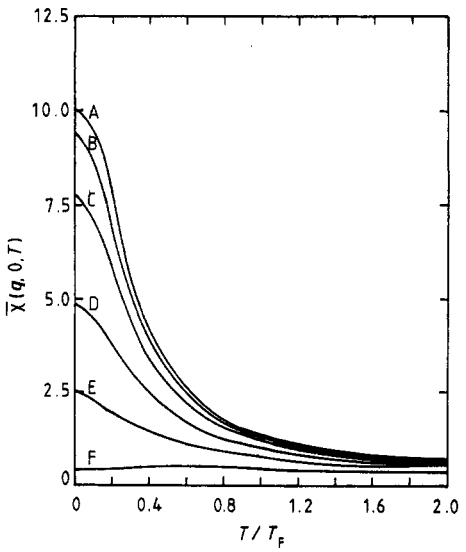

Figure 8. $\bar{\chi}(q, 0, T)$, evaluated in the ADH approach, versus T/T_F for different $|q|$-values with $S_{eff} = 10$: curve A, $|q| = 0.005$ au; curve B, $|q| = 0.4$ au; curve C, $|q| = 0.8$ au; curve D, $|q| = 1.4$ au; curve E, $|q| = 2.0$ au; curve F, $|q| = 3.0$ au.

in T. At very high temperatures it obeys the Curie law given by equation (45). The variation in $\bar{\chi}(\boldsymbol{q}, 0, T)$ with T becomes less important for large $\boldsymbol{q}$-values due to the decrease in the product $I\bar{\chi}^0(\boldsymbol{q}, 0, T)$ with increase in $\boldsymbol{q}$.

The bulk magnetic spin susceptibility is given by the limiting value of enhanced magnetic spin susceptibility $\chi(\boldsymbol{q}, \omega, T)$ at $\boldsymbol{q} = \omega = T = 0$. It is, therefore, given as

$$\chi(0, 0, 0) = \chi^{\mathrm{P}}/[1 - IN(E_{\mathrm{F}})]. \tag{56}$$

For V metal the experimental value of bulk magnetic susceptibility (Shimizu *et al* 1962, Akoh and Tasaki 1977, Kreissman and Callen 1954), which includes both the spin susceptibility and the contributions from the core and orbital motion, is 254.71×10^{-6} emu mol^{-1}. The orbital (Van Vleck) paramagnetism in the d-band metals is quite large (Kubo and Obata 1956, Hebborn and Place 1972) and in V metal it ranges from 75 to 200×10^{-6} emu mol^{-1} (Noer and Knight 1964, Clogston *et al* 1962, Yasui and Shimizu 1971, Place and Rhodes 1971). Therefore, the spin susceptibility is the difference between the experimental and orbital susceptibilities, i.e. $\chi_{\mathrm{spin}} = \chi_{\mathrm{exp}} - \chi_{\mathrm{orb}}$, and ranges from 54.71 to 179×10^{-6} emu mol^{-1}. In the theoretical estimation of $\chi_{\mathrm{spin}} = \chi(0, 0, 0)$ we take $I = 0.026$ Ryd for V metal from Janak (1977). It yields $\chi_{\mathrm{spin}} = 78.41 \times 10^{-6}$ emu mol^{-1} which falls well within the experimental range for spin susceptibility. With the above value of I the effective Stoner enhancement factor $S_{\mathrm{eff}} = 2.71$, which is in reasonable agreement with its experimental value (Knapp and Jones 1972) and other theoretical values (Janak 1977, Papaconstantopoulos *et al* 1977, Stenzel and Winter 1986). S^* and S^*_{dp} are found to be 1.86 and 0.85, respectively. If the depletion hole contribution is neglected, $\chi_{\mathrm{spin}} = 42.36 \times 10^{-6}$ emu mol^{-1} and the Stoner enhancement factor $S_{\mathrm{f}} = 1.46$, which are much less than their experimental values. Therefore in V metal the depletion hole plays a significant role.

Let us examine, in general, what type of d-band metal favours the existence of ferromagnetism in the present formalism. It is known that any element for which $IN(E_{\mathrm{F}}) \geqslant 1$ should be ferromagnetic in nature (Stoner 1954, Vosko and Perdew 1975). It has been shown that ferromagnetic substances have relatively large values for I but the ferromagnetism is basically determined by the DOS (Janak 1977). In the d-band metals the d-band resonant scattering, which depends upon $\mathrm{d}A_2/\mathrm{d}E$ (see equations (17)–(19)), gives a major contribution to the depletion hole and, therefore, is mainly responsible for the existence of ferromagnetism. The depletion hole contribution and hence $N(E_{\mathrm{F}})$ increase with decrease in W_{d}. Hence the present formalism predicts the possibility of ferromagnetism in the metals with a narrow d band. Watson and Bennett (1978) and Kakehashi (1981) calculated the d-band widths of 3d, 4d and 5d series of metals and found it to be minimum near the end of the 3d series (e.g. near Fe, Ni and Co) but quite large for the 4d and 5d series. Therefore, the product $IN(E_{\mathrm{F}})$ may be large enough for ferromagnetism to exist only at the end of 3d series and this favours the viewpoint of Janak (1977).

4. Conclusions

A model potential theory is developed for the temperature-dependent dynamical spin susceptibility $\chi^0(\boldsymbol{q}, \omega, T)$. The depletion hole is associated with the non-locality of the model potential and is studied by two different approaches: the EDH and ADH approaches. In the EDH approach both the $\boldsymbol{k}$- and the $\boldsymbol{q}$-dependence of the depletion hole contribution is included explicitly, but in the ADH approach the depletion hole contribution is summed

over all the occupied electronic states, which makes it temperature dependent. In this approach the depletion hole becomes independent of the vector k. The d-band contribution to the depletion hole has a resonant characteristic analogous to s–d hybridisation in the orthogonalised plane-wave pseudopotential theory (Harrison 1969) and gives a major contribution to it. $\chi^0(q, \omega, T)$, for V metal, is calculated in both approaches and strikingly the results are nearly the same. It supports the decoupling procedure given by Shaw and Harrison (1967) according to which the band structure and the overalap matrix element parts can, separately, be averaged in k-space. The reasonably good agreement between the calculated and experimental values of magnetic spin susceptibility, in the present formalism, emphasises the importance of the Bloch character of the conduction electrons. One should note that the present formalism is valid for all temperatures provided that one can calculate $E_F(T)$ reliably. In the end we would like to point out that the model potential theory can also be extended to the f-band metals provided that the pole at the f-band energy is properly handled.

Acknowledgments

I am grateful to Professor A J Freeman, Professor S K Sinha, Professor S K Joshi and Professor S Prakash for fruitful discussions. I am grateful to Dr S D Raj for rendering some help with the numerical computation. The financial support from Council of Scientific and Industrial Research, New Delhi (grant No 3 (656)/88. EMR. II), is acknowledged.

References

Akoh H and Tasaki A 1977 *J. Phys. Soc. Japan* **42** 791
Allan G, Lomer W H, Lowde R D and Windsor C G 1968 *Phys. Rev. Lett.* **20** 933
Animalu A O E 1973 *Phys. Rev.* B **8** 3542
Clogston A M, Gossard A C, Jaccarino V and Yafet Y 1962 *Phys. Rev. Lett.* **9** 262
Diamond J B 1972 *Int. J. Magn.***2** 241
Doniach S 1967 *Proc. Phys. Soc.* **91** 86
Doniach S and Engelberg S 1966 *Phys. Rev. Lett.* **17** 750
Doughlass D H 1975 *Superconductivity in d- and f-band Metals* vol 1 (New York: Plenum)
—— 1976 *Superconductivity in d- and f-band Metals* vol 2 (New York: Plenum)
Fay D and Appel J 1980 *Phys. Rev.* B **22** 3173
Harrison W A 1969 *Phys. Rev.* **181** 1036
Hebborn J E and March N H 1970 *Adv. Phys.* **19** 175
Hebborn J E and Place C M 1972 *Phys. Status Solidi* b **51** 359
Heine V and Abarenkov I V 1964 *Phil. Mag.* **9** 451
Horton G K and Maradudin A A 1981 *Dynamical Properties of Solids* vol III (Amsterdam: North-Holland)
Izuyama T, Kim J and Kubo R 1963 *J. Phys. Soc. Japan* **18** 1025
Janak J F 1977 *Phys. Rev.* B **16** 255
Johnson O 1980 *Phys. Status Solidi* b **99** 745
Jullien R , Beal-Monod M T and Coqblin B 1973 *Phys. Rev. Lett.* **30** 1057
—— 1974 *Phys. Rev.* B **9** 1441
Kaiser A B and Doniach S 1970 *Int. J. Magn.* **1** 11
Kakehashi Y 1981 *J. Phys. Soc. Japan* **50** 792
Knapp G S and Jones R W 1972 *Phys. Rev.* B **6** 1761
Kohn W and Sham L J 1965 *Phys. Rev.* **140** A1133
Kreissman C J and Callen H B 1954 *Phys. Rev.* **94** 837
Kubo R and Obata Y 1956 *J. Phys. Soc. Japan* **11** 547

Liu S H 1976 *Phys. Rev.* B **13** 3962
Löwde R D and Windsor C G 1970 *Adv. Phys.* **19** 813
Lynn J W and Mook H A 1981 *Phys. Rev.* B **23** 198
MacDonald A H 1981 *Phys. Rev.* B **24** 1130
Marshall W 1967 *Rendiconti della Scuola Internazionale di Fisica, 'Enrico Fermi', XXXII Corso* (New York: Academic)
Mook H A, Lynn J W and Nicklow R M 1973 *Phys. Rev. Lett.* **30** 556
Mook H A and Tocchetti D 1979 *Phys. Rev. Lett.* **43** 2029
Noer R J and Knight W D 1964 *Rev. Mod. Phys.* **36** 177
Papaconstantopoulos D A, Boyer L L, Klein B M, Williams A R, Moruzzi V L and Janak J F 1977 *Phys. Rev.* B **15** 4221
Pickett W E and Allen P B 1977 *Phys. Rev.* B **16** 3127
Place C M and Rhodes P 1971 *Phys. Status Solidi* b **47** 475
Rivier N and Zuckermann M J 1968 *Phys. Rev. Lett.* **21** 904
Shaw R W and Harrison W A 1967 *Phys. Rev.* **163** 604
Shimizu M 1981 *Phys. Lett.* **81A** 87
Shimizu M, Takahashi T and Katsuki A 1962 *J. Phys. Soc. Japan* **17** 1740
Singh J and Prakash S 1981 *J. Phys. F: Met. Phys.* **11** 2409
Singh R and Prakash S 1977 *Phys. Rev.* B **15** 5412
Singh R, Prakash S and Singh J 1981 *Phys. Rev.* B **23** 2357
Singh R, Singh J and Prakash S 1977 *Phys. Rev.* B **16** 4012
—— 1980 *J. Phys. F: Met. Phys.* **10** 1249
Singwi K S, Sjolander A, Tosi M P and Land R H 1970 *Phys. Rev.* B **1** 1044
Sokoloff J B 1978 *Phys. Rev.* B **17** 2380
Stearns M B 1973 *Phys. Rev.* B **8** 4383
—— 1978 *Phys. Today* **16** 34
Stenzel E and Winter H 1985 *J. Phys. F: Met. Phys.* **15** 1571
—— 1986 *J. Phys. F: Met. Phys.* **16** 1789
Stoner E C 1954 *Acta Metall.* **2** 260
Vosko S H and Perdew J P 1975 *Can. J. Phys.* **53** 1385
Watson R E and Bennett L H 1978 *Phys. Rev.* B **18** 6439
Yasui M and Shimizu M 1971 *J. Phys. Soc. Japan* **31** 378