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On the influence of spin fluctuations on the superconducting transition temperatures of transition metals

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Abstract. We develop an *ab initio* theory for the combined influence of phonons and spin fluctuations on the superconducting transition temperatures, T_c, of transition metals. The ingredients of the Eliashberg equations, like the electronic structure, the spin fluctuation spectrum and the coupling function, are calculated in the local density functional–random phase approximation without introducing adjustable parameters, whereas the spin-independent part of the Coulomb interaction is treated using a McMillan parameter. We describe the steps involved in transforming the Eliashberg equations into a numerically tractable form without resorting to jellium model-like assumptions. For the case of vanadium we find that spin fluctuations reduce T_c substantially below the value corresponding to the pure phonon mechanism.

1. Introduction

Most of the theoretical investigations of superconducting transition temperatures, T_c, in the past aimed at an *ab initio* treatment of the electron–phonon coupling mechanism (e.g. Gaspari and Gyorffy 1972, Gomersall and Gyorffy 1974, Butler *et al* 1976, Papaconstantopoulos *et al* 1977, Winter *et al* 1978, Rietschel 1978, Glötzel *et al* 1979, Jarlborg *et al* 1983). Band-structure work yielded both the electronic quantities and the electron–phonon coupling matrix elements in rigid muffin-tin approximation (RMTA) (Mott and Jones 1936). Efforts to go beyond the RMTA—especially important in the case of simple metals—have also been undertaken (Winter 1981). The phonon modes have been obtained using shell models (Weber 1973) or in some special cases via microscopic calculations (e.g. Varma and Weber 1979, Ho *et al* 1982, Weber 1984). In this way reliable phonon kernels for the Eliashberg equations of both the normal and the anomalous self-energies became available. The Coulomb interactions on the other hand have been taken into account in a crude manner through the use of McMillan's parameter μ^*, whose value was put equal to something like 0.13 (McMillan 1968). The largest discrepancies between the results of these kinds of theories and experiment among the systems investigated turned out to occur for vanadium and its compounds.

Later on a correlation between the degree of failure in predicting the correct T_c and the value of the static homogeneous spin susceptibility was pointed out (Rietschel and Winter 1979). This observation motivated the effort to treat the coupling of the electrons

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to spin fluctuations on the same footing as the phonon mechanism, as Berk and Schrieffer (1966) had previously done for Pd. A substantial reduction of T_c below the value resulting from the phonon mechanism alone has indeed been found for V and some of its compounds (Rietschel *et al* 1980).

However, neglecting band-structure effects and the crystalline lattice, this work treats the spin fluctuation mechanism in jellium model approximation involving the introduction of parameters fitted to the experimental Stoner enhancement and the spin fluctuation contribution to the effective mass of the electrons. It should be mentioned that it is hard to extract the latter quantity unambiguously from experiment. Especially in the case of Pd this kind of theory proved unable to explain the observed low value of the electronic mass enhancement satisfactorily.

In previous work we developed a formalism for calculating the wavevector- and frequency-dependent spin susceptibility of paramagnetic metals in local density functional–random phase approximation (LDA-RPA) (Stenzel and Winter 1985). In our application to V and Pd (Stenzel *et al* 1988) we calculated the fluctuation spectra, the electron spin fluctuation coupling matrix elements and the electronic mass enhancements. We obtained small values for the quantities $(m^{*sp} - m)/m$ (0.16 for Pd and 0.11 for V), numbers that are compatible with experiment.

In this paper we present an *ab initio* T_c theory, describing the combined influence of phonons and spin fluctuations within LDA-RPA and implementing the Eliashberg equations with the effects of the band structure and the crystalline lattice also in the spin fluctuation parts. The spin-independent part of the Coulomb interaction on the other hand is treated using a McMillan parameter, μ^*. We discuss applications on vanadium. The paper is organised as follows. In section 2 we set up the Eliashberg equations in terms of explicit expressions for the phonon and the spin fluctuation kernels. Further details concerning this point are given in the appendices 1 and 2. Section 3 is devoted to the display and the discussion of the phonon and the spin fluctuation excitation spectra, whereas section 4 sheds some light on the problems encountered in and the methods employed to deal with the numerical aspects. Results for the normal self-energy of V are presented in section 5 and in section 6 we discuss the numerical solution of the gap equation. We conclude with a short summary in section 7.

2. The derivation of the linearised Eliashberg equations

For the part of the anomalous self-energy, Σ^{+-sp}, of the electrons that is due to their interaction with spin fluctuations we use the following expression:

$$\Sigma^{+-sp}(\boldsymbol{r}, \boldsymbol{r}', \varepsilon_n) = \frac{-3}{i\beta} \sum_{\varepsilon_m} \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \, K^s_{xc}(\boldsymbol{r}) \chi^s(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon_m - \varepsilon_n)$$

$$\times K^s_{xc}(\boldsymbol{r}') \bar{g}(\boldsymbol{r}, \boldsymbol{r}_1, \varepsilon_m) \Sigma^{+-}(\boldsymbol{r}_1, \boldsymbol{r}_2; \varepsilon_m) g(\boldsymbol{r}_2, \boldsymbol{r}', \varepsilon_m). \tag{2.1}$$

Here, g and $\bar{g}(\boldsymbol{r}, \boldsymbol{r}_1, \varepsilon_m) = g(\boldsymbol{r}_1, \boldsymbol{r}, -\varepsilon_m)$ are the one-particle Green functions of the normal state, χ^s is the spin fluctuation propagator and K^s_{xc} is the electron–spin fluctuation coupling potential (Stenzel and Winter 1985). The ε_n and ε_m are Fermi–Matsubara frequencies. As a consequence of the broken translational invariance, the propagators depend on two real-space coordinates.

Restricting ourselves for the sake of simplicity of notation to systems with one atom in the unit cell, we perform a lattice Fourier transformation on equation (2.1), that is we use the $\boldsymbol{k}, \boldsymbol{q}$ representation of Zak (1972). We obtain

$$\Sigma_{\boldsymbol{q}}^{+-\mathrm{sp}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n) = \frac{-3}{\mathrm{i}\beta} \sum_{\varepsilon_m} \int \mathrm{d}\boldsymbol{\rho}_1 \, \mathrm{d}\boldsymbol{\rho}_2 \int \frac{\mathrm{d}\boldsymbol{k}}{\Omega_{\mathrm{BZ}}} K_{\mathrm{xc}}^{\mathrm{s}}(\boldsymbol{\rho}) \chi_{\boldsymbol{q}-\boldsymbol{k}}^{\mathrm{s}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_m - \varepsilon_n) K_{\mathrm{xc}}^{\mathrm{s}}(\boldsymbol{\rho}')$$

$$\times \bar{g}_{\boldsymbol{k}}(\boldsymbol{\rho}, \boldsymbol{\rho}_1, \varepsilon_m) \, \Sigma_{\boldsymbol{k}}^{+-}(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2; \varepsilon_m) g_{\boldsymbol{k}}(\boldsymbol{\rho}_2, \boldsymbol{\rho}', \varepsilon_m). \tag{2.2}$$

In equation (2.2) the local coordinates $\boldsymbol{\rho}, \boldsymbol{\rho}'$ are restricted to a Wigner–Seitz (ws) cell and the momenta $\boldsymbol{q}, \boldsymbol{k}$ are confined to the first Brillouin zone (BZ) with volume Ω_{BZ}.

The lattice structure of the system allows for the following representation of g:

$$g_{\boldsymbol{q}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n) = \sum_{\nu} \Psi_{\boldsymbol{q}\nu}(\boldsymbol{\rho}) \frac{1}{\varepsilon_n - \Sigma_{\boldsymbol{q}\nu}(\varepsilon_n) - \varepsilon_{\boldsymbol{q}\nu}} \Psi_{\boldsymbol{q}\nu}^*(\boldsymbol{\rho}'). \tag{2.3}$$

Here, the Ψ are one-particle wavefunctions, which are simultaneously eigenfunctions of the lattice translation operators, ν is the band index and the $\varepsilon_{\boldsymbol{q}\nu}$ are the band energies. We assume that similar representations hold for other quantities approximately as well. Starting from some quantity $A_{\boldsymbol{q}}(\boldsymbol{\rho}, \boldsymbol{\rho}', \varepsilon_n)$ we define the transform $\tilde{A}$ via the following relation:

$$\tilde{A}_{\boldsymbol{q}\nu}(\varepsilon_n) = \int \mathrm{d}\boldsymbol{\rho} \int \mathrm{d}\boldsymbol{\rho}' \, \Psi_{\boldsymbol{q}\nu}^*(\boldsymbol{\rho}) A_{\boldsymbol{q}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n) \Psi_{\boldsymbol{q}\nu}(\boldsymbol{\rho}'). \tag{2.4}$$

Applying the transformation (2.4) on equation (2.2) we obtain after some straightforward manipulations

$$\tilde{\Sigma}_{\boldsymbol{q}\nu}^{+-\mathrm{sp}}(\varepsilon_n) = \frac{-3}{\mathrm{i}\beta} \sum_{\varepsilon_m, \bar{\nu}} \int \frac{\mathrm{d}\boldsymbol{k}}{\Omega_{\mathrm{BZ}}} M^{\mathrm{s}}(\boldsymbol{q}\nu, \boldsymbol{k}\bar{\nu})^* \times \chi_{\boldsymbol{q}-\boldsymbol{k}}^{\mathrm{s}}(\varepsilon_m - \varepsilon_n) \times M^{\mathrm{s}}(\boldsymbol{k}\bar{\nu}, \boldsymbol{q}\nu) \tilde{\Sigma}_{\boldsymbol{k}\bar{\nu}}^{+-}(\varepsilon_m)$$

$$\times \{[\mathrm{Im}(\varepsilon_m + \tilde{\Sigma}_{\boldsymbol{k}\bar{\nu}}(\varepsilon_m))]^2 + [\varepsilon_{\boldsymbol{k}\bar{\nu}} + \mathrm{Re}\, \tilde{\Sigma}_{\boldsymbol{k}\bar{\nu}}(\varepsilon_m) - \varepsilon_{\mathrm{F}}]^2\}^{-1}. \tag{2.5}$$

Here, $\tilde{\Sigma}_{\boldsymbol{k}\bar{\nu}}$ is the normal self-energy and the matrix elements of the spin fluctuation–electron coupling function, $M^{\mathrm{s}*} \times \chi^{\mathrm{s}} \times M^{\mathrm{s}}$, are defined through the relation:

$$M^{\mathrm{s}}(\boldsymbol{q}\nu, \boldsymbol{k}\bar{\nu})^* \times \chi_{\boldsymbol{q}-\boldsymbol{k}}^{\mathrm{s}}(\varepsilon_m - \varepsilon_n) \times M^{\mathrm{s}}(\boldsymbol{k}\bar{\nu}, \boldsymbol{q}\nu)$$

$$= \int \mathrm{d}\boldsymbol{\rho} \int \mathrm{d}\boldsymbol{\rho}' \, \Psi_{\boldsymbol{q}\nu}^*(\boldsymbol{\rho}) K_{\mathrm{xc}}^{\mathrm{s}}(\boldsymbol{\rho}) \Psi_{\boldsymbol{k}\bar{\nu}}(\boldsymbol{\rho}) \chi_{\boldsymbol{q}-\boldsymbol{k}}^{\mathrm{s}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n - \varepsilon_m)$$

$$\times \Psi_{\boldsymbol{k}\bar{\nu}}^*(\boldsymbol{\rho}') K_{\mathrm{xc}}^{\mathrm{s}}(\boldsymbol{\rho}') \Psi_{\boldsymbol{q}\nu}(\boldsymbol{\rho}'). \tag{2.6}$$

An explicit expression for $M^{\mathrm{s}*} \times \chi^{\mathrm{s}} \times M^{\mathrm{s}}$ in terms of the coefficients of the local, angular momentum decomposition of Ψ and χ^{s} is given in appendix 1.

In the form of relation (2.5) the equation for $\tilde{\Sigma}^{+-}$ is a matrix equation in the Matsubara frequencies and the band indices and a three-dimensional integral equation

in the momentum variable. To simplify things, we define the quantity $\Delta(\varepsilon_n, x)$ depending on the continuous energy variable x via the relation

$$\Delta(\varepsilon_n, x) = \sum_\nu \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu}) \tilde{\Sigma}^{+-}_{q\nu}(\varepsilon_n) \Big(\sum_\nu \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu}) \Big)^{-1}. \tag{2.7}$$

$\Delta(\varepsilon_n, x)$ is an average of Σ^{+-} over the momenta $\boldsymbol{q}$ and the bands ν at energy x. Inserting the expression (2.7) into equation (2.5) we get

$$\Delta^{\mathrm{sp}}(\varepsilon_n, x) = \sum_m \int \mathrm{d}y \, K^{\mathrm{sp}}(x, y, \varepsilon_n, \varepsilon_m) \Delta(\varepsilon_m, y) \tag{2.8}$$

whereby the kernel, K^{sp}, of the spin fluctuation coupling mechanism is defined by the relation

$$\begin{aligned} K^{\mathrm{sp}}(x, y, \varepsilon_n, \varepsilon_m) = {} & \frac{-3}{\beta n(x)} \sum_{\nu,\bar{\nu}} \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu}) \int \frac{\mathrm{d}\boldsymbol{k}}{\Omega_{\mathrm{BZ}}} \delta(y - \varepsilon_{k\bar{\nu}}) M^{\mathrm{s}*}(\boldsymbol{q}\nu, \boldsymbol{k}\bar{\nu}) \\ & \times \chi^{\mathrm{s}}_{q-k}(\varepsilon_m - \varepsilon_n) \times M^{\mathrm{s}}(\boldsymbol{k}\bar{\nu}, \boldsymbol{q}\nu) \{ [\mathrm{Im}(\varepsilon_m + \tilde{\Sigma}_{\bar{\nu}}(\varepsilon_m, y))]^2 \\ & + [y - \varepsilon_{\mathrm{F}} + \mathrm{Re}\, \tilde{\Sigma}_{\bar{\nu}}(\varepsilon_m, y)]^2 \}^{-1}. \end{aligned} \tag{2.9}$$

In deriving equations (2.8) and (2.9) we approximated both the normal and the anomalous self-energy on the RHS of equation (2.5) with their averages over the energy shells y. This may be considered as a generalisation of the 'dirty limit' approximation frequently applied in work dealing with the phonon mechanism alone. This approximation is strongly supported by the results of Peter *et al* (1982), who investigated the influence of Fermi-surface anisotropies on the superconducting transition temperatures of some d-band transition metals and found only minor effects.

To complete our setting up of the gap equation, we add the following expression for the phonon kernel used in the present calculation and derived, for example, by Glötzel *et al* (1979):

$$\tilde{K}^{\mathrm{phon}}(\varepsilon_n, \varepsilon_m) = (\pi/\beta) \lambda(\varepsilon_m - \varepsilon_n) / |\varepsilon_m + \mathrm{Im}\, \tilde{\Sigma}(\varepsilon_m, \varepsilon_{\mathrm{F}})| \tag{2.10}$$

with

$$\lambda(\varepsilon_m) = 2 \int_0^\infty \mathrm{d}\omega \, \frac{\alpha^2 F(\omega) \omega}{\omega^2 - \varepsilon_m^2} \tag{2.11}$$

and

$$\begin{aligned} \alpha^2 F(\omega) = {} & \frac{1}{2Mn(\varepsilon_{\mathrm{F}})\omega} \sum_{\nu_1,\nu_2,\lambda} \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \int \frac{\mathrm{d}\boldsymbol{k}}{\Omega_{\mathrm{BZ}}} \delta(\varepsilon_{\mathrm{F}} - \varepsilon_{q\nu_1}) \delta(\varepsilon_{\mathrm{F}} - \varepsilon_{k\nu_2}) \delta(\omega - \omega_{q-k,\lambda}) \\ & \times [\boldsymbol{M}^{\mathrm{ph}}(\boldsymbol{q}\nu_1, \boldsymbol{k}\nu_2)^* \cdot \boldsymbol{e}^*_{q-k,\lambda}] [\boldsymbol{M}^{\mathrm{ph}}(\boldsymbol{q}\nu_1, \boldsymbol{k}\nu_2) \cdot \boldsymbol{e}_{q-k,\lambda}] \end{aligned} \tag{2.12}$$

with

$$\boldsymbol{M}^{\mathrm{ph}}(\boldsymbol{q}\nu_1, \boldsymbol{k}\nu_2) = \int \mathrm{d}\boldsymbol{\rho} \, \Psi^*_{q\nu_1}(\boldsymbol{\rho}) \nabla V(\boldsymbol{\rho}) \Psi_{k\nu_2}(\boldsymbol{\rho})$$

whereby $\tilde{K}^{\mathrm{phon}}$ is defined through

$$\tilde{K}^{\mathrm{phon}}(\varepsilon_n, \varepsilon_m) = \int \mathrm{d}y \, K^{\mathrm{phon}}(\varepsilon_{\mathrm{F}}, y, \varepsilon_n, \varepsilon_m).$$

Here, $\boldsymbol{e}_{q\lambda}$ and $\omega_{q\lambda}$ are the phonon polarisation vectors and frequencies, respectively. As

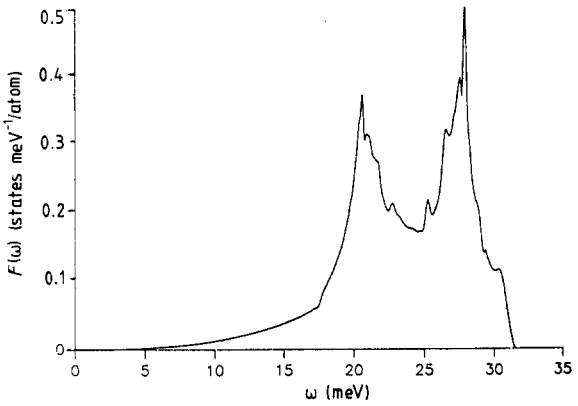

Figure 1. The phonon density of states of vanadium calculated using the double shell model of Weber (1973).

we use the RMTA for electron–phonon coupling, ∇V is the gradient of the crystalline electron potential in muffin-tin form (Gomersall and Gyorffy 1974). Owing to the limited energy range of the phonon spectrum ($\omega_{max} = 32$ meV) the variable x has been confined to ε_F. Further details are given in appendix 2.

Collecting equations (2.8) to (2.10) the gap equation finally reads

$$\Delta(\varepsilon_n, x) = \sum_m \int dy \Big[K^{phon}(x, y, \varepsilon_n, \varepsilon_m) + K^{sp}(x, y, \varepsilon_n, \varepsilon_m) - \mu^* \Big] \Delta(\varepsilon_m, y). \tag{2.13}$$

In equation (2.13) the spin-independent part of the Coulomb interaction has been taken into account via the McMillan parameter μ^*, a procedure that may be justified if the phonon and the spin fluctuation spectra are clearly separated from the energy range where appreciable charge density fluctuation amplitudes occur.

3. The fluctuation spectra

The phonon spectrum has been obtained using the double shell model of Weber (1973) and fitting its parameters at first to the measured phonon dispersions of the similar system Nb. With the help of a rescaling factor, which turned out to correspond up to 5% with the V–Nb atom mass ratio, the resulting shell model phonon density of states (DOS) has been fitted to the measured one afterwards. The phonon spectrum (figure 1) exhibits the usual transverse and longitudinal phonon peaks and extends up to 32 meV.

The spin fluctuation spectrum has been taken from the work of Stenzel *et al* (1988), who calculated the full matrix $\hat{\chi}$ defined in equation (A1.3) and needed for establishing the kernel, K^{sp}, of the gap equation. To give a general impression of its behaviour we draw the diagonal part, $\mathrm{Im}\,\chi^s(\boldsymbol{q}, \boldsymbol{q}; \omega)$, of the double real-space Fourier transform of its imaginary part in figure 2 as a function of frequency and for some wavevectors $\boldsymbol{q}$ in (100) direction as parameters. $\mathrm{Im}\,\chi^s(\boldsymbol{q}, \boldsymbol{q}; \omega)$ is defined through the relation

$$\mathrm{Im}\,\chi^s(\boldsymbol{q}, \boldsymbol{q}; \omega) = \int d\boldsymbol{\rho} \int d\boldsymbol{\rho}'\, e^{-i\boldsymbol{q}(\boldsymbol{\rho}-\boldsymbol{\rho}')}\, \mathrm{Im}\,\chi^s_{\boldsymbol{q}}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \omega). \tag{3.1}$$

The sharp structures at small wavevectors and frequencies are due to intraband transitions within bands 2 and 3, which build up the Fermi surface. More and more interband

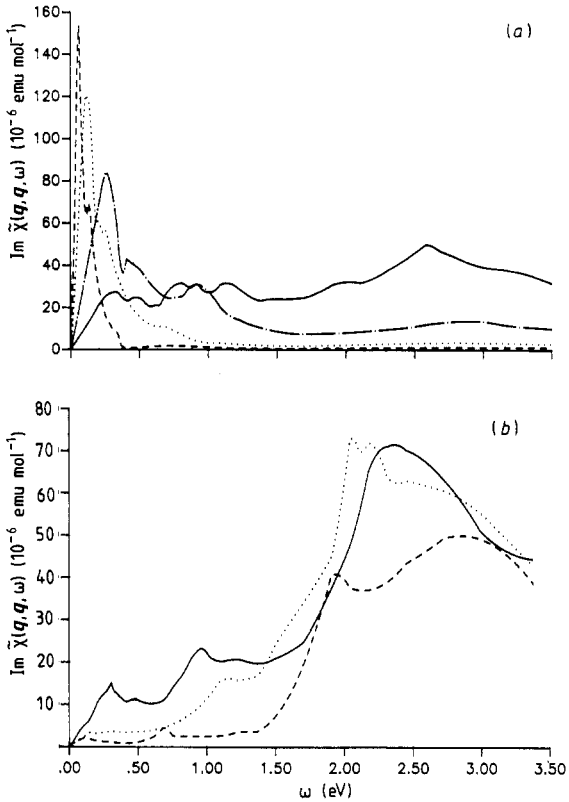

Figure 2. The spin fluctuation spectrum of V, Im $\tilde{\chi}^{sp}(q, q, \omega)$, as a function of frequency ω for some q-values in the (100)-direction (q is in units of $2\pi/a$) as calculated by Stenzel *et al* (1988): (*a*) $|q| = 0.05$ (- - -), $|q| = 0.1$ (·····), $|q| = 0.2$ (-·-·-), $|q| = 0.4$ (——); (*b*) $|q| = 0.6$ (——), $|q| = 0.8$ (· · ·), $|q| = 1.0$ (– – –).

transitions play a role on increasing q and the energy extent of the curves increases, while their amplitudes diminish and the structures get washed out. As the subsequent investigations of this paper show, spin fluctuations up to about 5 eV influence T_c significantly. Electron loss spectrocopy (ELS) measurements (Simmons and Scheibner 1972, Misell and Atkins 1972, Wehenkel and Gauthé 1975) on the other hand show that the density fluctuation spectrum peaks at about 20 eV, showing extremely broad features. Its main amplitudes occur at energies appreciably above 5 eV. In the light of these findings our approximation to treat the spin-independent part of the Coulomb interaction via μ^* seems to be justified.

4. Numerical aspects

Self-consistent Korringa–Kohn–Rostoker (KKR) band-structure calculations have been performed to obtain the six lowest conduction bands of V. Subsequently, the Bloch state coefficients, $c^{(k)}_{lm;\nu}$ and the energy eigenvalues, $\varepsilon_{k\nu}$, have been evaluated on a dense equidistant k-mesh (up to 100 k-points per ray) along 136 rays approximately uniformly

distributed over the irreducible wedge of the Brillouin zone (IWBZ), emanating from the Γ-point and ending at the BZ boundary. This mesh is used to subdivide the IWBZ into a space-filling network of small volume elements, $P^i_{j'}$ (compare Winter *et al* 1988).

In order to evaluate the kernels of the gap equation (equations (2.9) and (2.12)) we need to spot the zeros of the arguments of δ-functions like $\delta(x - \varepsilon_{q\nu})$ for wavevectors $\boldsymbol{q}$ within the IWBZ. Integrals like $\int \mathrm{d}\boldsymbol{q}\, \delta(x - \varepsilon_{q\nu})$ are piecewise performed over all the volume elements $P^i_{j'}$ that contribute. We employ thereby techniques similar to those explicitly described by Winter *et al* (1988). The factors multiplying the δ-functions are replaced by their averages over the corners of each individual volume element $P^i_{j'}$. In the case of the coupling functions $M^{s*} \times \chi^s \times M^s$ (equation (A1.5)) and the Bloch state coefficients (equation (A2.1)), averaging over larger regions of the IWBZ proved sufficient. For this purpose the IWBZ has been subdivided into 40 regions of approximately constant volume. The integration of $\boldsymbol{q}$ and $\boldsymbol{k}$ over the whole BZ instead of the IWBZ has been achieved by applying the 48 O_h point group symmetry operations on the factors of the δ-functions, thereby exploiting the symmetries of the $\varepsilon_{k\nu}$ and the $c^{(k)}_{lm;\nu}$.

5. The normal self-energy and the electron mass enhancement

In analogy to equation (2.7) we define a quantity $\Sigma(\varepsilon_n, x)$ as the average of $\Sigma_{q\nu}(\varepsilon_n)$ over the energy shells x:

$$\tilde{\Sigma}(\varepsilon_n, x) = \sum_\nu \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu})\, \Sigma_{q\nu}(\varepsilon_\nu) \Big(\sum_\nu \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu}) \Big)^{-1}. \tag{5.1}$$

Using the standard derivation for the phonon case we obtain

$$\Sigma^{\mathrm{phon}}(\varepsilon_n, \varepsilon_{\mathrm{F}}) = \frac{\mathrm{i}\pi}{\beta} \sum_m \lambda(\varepsilon_m - \varepsilon_n)\, \mathrm{sgn}(\varepsilon_m/\mathrm{i}) \tag{5.2}$$

and for the mass enhancement of the electrons due to their interactions with the phonons we get

$$\frac{m^{*\,\mathrm{phon}}}{m} - 1 = 2\int_0^\infty \mathrm{d}\omega\, \alpha^2 F(\omega)/\omega. \tag{5.3}$$

The quantities $\lambda(\varepsilon_m)$ and $\alpha^2 F(\omega)$ are defined through equations (2.11) and (2.12), respectively. The techniques used in the evaluation of the normal self-energy are the same as those sketched in section 4 in connection with the calculation of the kernels. We obtain

$$\frac{m^{*\,\mathrm{phon}}}{m} - 1 = 1.03$$

a number that is in the range of previously published results (Butler *et al* 1977, Collela and Batterman 1970).

The equation for the normal self-energy due to the electron–spin fluctuation coupling mechanism reads in the weak coupling limit:

$$\tilde{\Sigma}^{\mathrm{sp}}(\varepsilon_n, x) = \frac{-3}{\beta n(x)} \sum_m \sum_{\nu,\bar{\nu}} \int \frac{\mathrm{d}\boldsymbol{q}}{\Omega_{\mathrm{BZ}}} \int \frac{\mathrm{d}\boldsymbol{k}}{\Omega_{\mathrm{BZ}}} \delta(x - \varepsilon_{q\nu}) M^{s^*}(\boldsymbol{q}\nu, \boldsymbol{k}\bar{\nu})$$
$$\times \chi^s_{q-k}(\varepsilon_m - \varepsilon_n) \times M^s(\boldsymbol{k}\bar{\nu}, \boldsymbol{q}\nu)/(\varepsilon_m - \varepsilon_{k\bar{\nu}} + \varepsilon_{\mathrm{F}}). \tag{5.4}$$

As a starting point for the calculation of the low-temperature effective mass we use the following formula:

$$\frac{m^*}{m} = \frac{-2}{\pi n(\varepsilon_F)} \int d\boldsymbol{r}\, d\boldsymbol{r}'\, \mathrm{Im}\, g(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon_F) \left(\delta(\boldsymbol{r} - \boldsymbol{r}') - \frac{\partial}{\partial \varepsilon} M(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon) \Big|_{\varepsilon = \varepsilon_F} \right). \tag{5.5}$$

Equation (5.5) has been derived by Luttinger (1960), Luttinger and Ward (1960) and Riedel (1968). In the way written above it may be applied to the case of broken translational symmetry. Approximating Im g by its band-structure value we end up with the following relation:

$$\frac{m^{*\mathrm{sp}}}{m} - 1 = \mathrm{i}[\mathrm{Im}\, \tilde{\Sigma}^{\mathrm{sp}}(\varepsilon_1, \varepsilon_F) - \mathrm{Im}\, \tilde{\Sigma}^{\mathrm{sp}}(\varepsilon_0, \varepsilon_F)]/(\varepsilon_1 - \varepsilon_0) \tag{5.6}$$

with

$$\varepsilon_n = (\pi/\beta)\, \mathrm{i}(2n + 1).$$

We get

$$\lambda_{\mathrm{sp}} = (m^{*\mathrm{sp}}/m) - 1 = 0.14.$$

Use has thereby been made of the analytical properties of $\tilde{\Sigma}$ and its nearly linear energy dependence near ε_F.

This value is sufficiently close to the number recently obtained by Stenzel *et al* (1988) ($\lambda_{\mathrm{sp}} = 0.11$) using slightly different numerical methods, whereby one should keep in mind that in the present calculation we did not subtract off the single bubble double-counting term (Riedel 1968).

The real part of $\tilde{\Sigma}^{\mathrm{sp}}$ (real in the complex Matsubara frequency representation) turns out to be insignificant.

The influence of Green function renormalisation effects on $m^{*\mathrm{sp}}$, neglected in the present treatment, have been investigated by Fay *et al* (1988). They find considerable effects for highly Stoner-enhanced systems with λ_{sp} in the range of 3. In the case of the moderately Stoner-enhanced metal V, we expect them to be of less importance.

6. The solution of the gap equation

The task is to find the highest temperature $T = T_c$ at which the linearised gap equation (equation (2.8)) has a non-trivial solution for Δ. In contrast to the pure phonon mechanism, the spin fluctuation kernel introduces the energy variables x and y. A possible method to treat this additional degree of freedom consists of subdividing the $x(y)$ space into intervals, I_n, defined through the relation

$$I_n: \qquad x_n - \Delta e(n) \leqslant x \leqslant x_n + \Delta e(n). \tag{6.1}$$

A similar relation holds for y.

Within the intervals I_n, $\Delta(\varepsilon_n, x)$ is approximated by its average value

$$\Delta(\varepsilon_m, n) = \frac{1}{2\Delta e(I_n)} \int_{x_n - \Delta e(I_n)}^{x_n + \Delta e(I_n)} dx\, \Delta(\varepsilon_m, x). \tag{6.2}$$

The choice of the number and the sizes of the regions I_n depend on the behaviour of K^{sp}

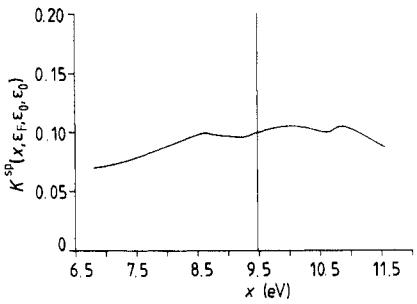

Figure 3. An illustration of the dependence of the spin kernel $K^{sp}(x, y, \varepsilon_n, \varepsilon_m)$ on the energy variable x. Drawn is the quantity $K^{sp}(x, \varepsilon_F, \varepsilon_0, \varepsilon_0)$ for x in a range of about 4 eV around the Fermi energy.

of the system in question. In this way we cast the gap equation into the form of a matrix equation in both the Matsubara frequencies and the indices n of the energy intervals I_n.

Our investigations show that in the case of V the situation is especially simple. First of all—due to the denominator $1/[\mathrm{Im}(\varepsilon_m + \tilde{\Sigma})^2 + (y + \mathrm{Re}\,\tilde{\Sigma})^2]$ in equation (2.9)—K^{sp} decreases sufficiently fast with increasing y for x-values not too far away (some eV) from the Fermi energy. Its dependence on x on the other hand is rather smooth. To visualise this behaviour, we draw the quantity $K^{sp}(x, \varepsilon_F, \varepsilon_0, \varepsilon_0)$ in figure 3 as a function of x within an interval of about 4 eV in the vicinity of ε_F. Because this energy range turns out to determine predominantly T_c, it therefore seems reasonable to replace $\Delta(\varepsilon_n, x)$ on the LHS of equation (2.13) with $\tilde{\Delta}(\varepsilon_n) = \Delta(\varepsilon_n, \varepsilon_F)$. On the RHS we replace $\Delta(\varepsilon_m, y)$ with $\tilde{\Delta}(\varepsilon_m)$ and integrate the kernels over their variable y, ending up with the following simplified form of the gap equation:

$$\tilde{\Delta}(\varepsilon_n) = \sum_m [\tilde{K}^{\mathrm{phon}}(\varepsilon_n, \varepsilon_m) + \tilde{K}^{sp}(\varepsilon_n, \varepsilon_m) - \mu^*]\tilde{\Delta}(\varepsilon_m) \tag{6.13}$$

with

$$\tilde{K}^{sp}(\varepsilon_n, \varepsilon_m) = \int \mathrm{d}y\, K^{sp}(\varepsilon_F, y, \varepsilon_n, \varepsilon_m). \tag{6.4}$$

The y-integration in equation (6.4) comprised the energy range of the six lowest conduction bands, whereby the contributions of bands 4 to 6 turned out to be rather insignificant.

In figure 4 we exhibit $\tilde{K}^{sp}(\varepsilon_n, \varepsilon_m)$ as a function of ε_m for some ε_n as parameters. The contributions coming from combinations of bands 2 and 3 are drawn in figure 4(a), whereas figure 4(b) shows the total spin kernel $\tilde{K}^{sp}$. $\tilde{K}^{sp}(\varepsilon_n, \varepsilon_m)$ drops sharply with both increasing ε_n and ε_m. As $\tilde{K}^{sp}$ is a smooth function of these variables, it is easy to interpolate it, using the interpolation scheme of Stör and Bulirsch (1980) on any discrete Matsubara frequency mesh determined by the actual temperature T at which a solution of the gap equation is sought. In our calculations we included Matsubara frequencies up to $\varepsilon_{\max} = 12$ eV. Up to 0.4 eV we took account of all ε_m, whereas the energy range between 0.4 eV and $\varepsilon_{\max}$ has been subdivided into intervals, I_κ. Within each interval, I_κ, we replaced $\tilde{\Delta}$ with its average value and summed $\tilde{K}^{sp}$ over the Matsubara frequencies contained in I_κ. The maximum number of intervals I_κ amounted to 40.

The choice for the employed value of μ^* comes from the following argument. In niobium the amplitudes of the spin fluctuations seem to be rather small. The value of μ^* in this system is therefore likely to be mainly attributable to the spin-independent part of the Coulomb interaction. This quantity in turn is determined by the coupling of the

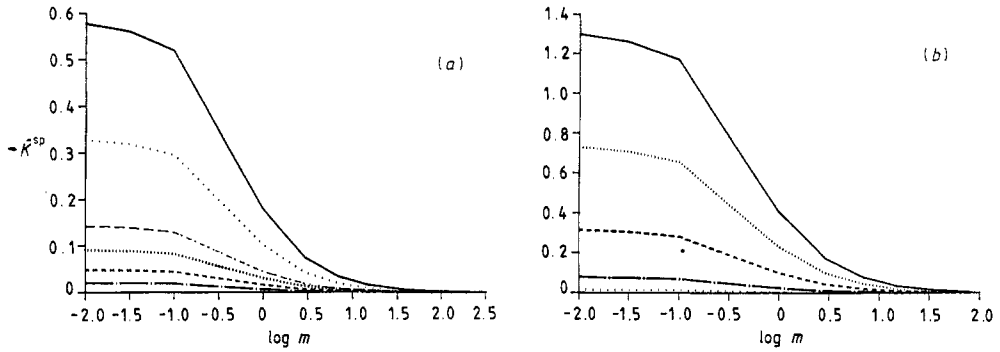

Figure 4. The spin fluctuation kernel, $\tilde{K}^{sp}(\varepsilon_n, \varepsilon_m)$, as a function of frequency ε_m for some ε_n values at $T = 10$ K. (*a*) Intraband contributions: band 2, $n = 1$ (·····), $n = 4$ (- - -), $n = 8$ (—·—); band 3, $n = 1$ (——), $n = 4$ (· · · ·), $n = 8$ (– – –). (*b*) The total spin fluctuation kernel used in the present calculations: $n = 1$ (———), $n = 4$ (·····), $n = 8$ (- - -), $n = 18$ (—·—), $n = 40$ (· · · ·).

Table 1. The calculated superconducting transition temperature T_c of V as a function of the cut-off parameter ε_{max}, ignoring and including spin fluctuations.

ε_{max} (eV)	μ^*	T_c ignoring spin fluctuations (K)	T_c including spin fluctuations (K)
$0.19 \simeq 5\omega_{Debye}$	0.13	19.43	8.43
$0.95 \simeq 25\omega_{Debye}$	0.15	19.48	9.23
$9.1 \simeq 240\omega_{Debye}$	0.225	19.46	9.48
$12 \simeq 320\omega_{Debye}$	0.243	19.44	9.48

electrons to the density fluctuations. As the experiments of Wehenkel and Gauthé (1975) and Misell and Atkins (1973) show, the fluctuation spectra of V and Nb are similar, which is hardly surprising in view of the fact that these substances are in the same column of the periodic table. It therefore seems reasonable to use the number 0.13 for μ^* at a cut-off of $5\omega_{Debye}$, proposed by McMillan (1968) in the case of Nb, for V as well. Because the purpose of the present paper is to demonstrate the importance of the spin fluctuations, a more profound investigation of the role of the spin-independent part of the Coulomb interaction will be postponed to future work. To obtain T_c we applied the procedure devised by Bergmann and Rainer (1973). The gap equation is cast into the form of an eigenvalue problem and the kernels are augmented by a pair breaking parameter, p. For a given value of p the highest temperature, $T_c(p)$, is sought for which a solution of the gap equation with eigenvalue $\lambda = 1$ exists. An iterative procedure in a two-dimensional subspace is thereby applied. If this procedure is carried through for a couple of p-values, the desired transition temperature, $T_c = T_c(p = 0)$, can be found by extrapolation. To test the influence of the frequency cut-off, ε_{max}, on T_c we performed the calculations for values of ε_{max} below 12 eV as well. Our results are collected in table 1.

To explore the precise cut-off dependence of μ^* we solved the gap equation switching off $\tilde{K}^{sp}$ at first. Then μ^* has been adjusted such that the calculated transition temperatures, T_c^{phon}, were independent of ε_{max}. Column 2 of table 1 shows the corresponding values. They scale nearly according to the following rule, derived by Bogoliubov (1958):

$$\mu^*(\varepsilon_{max}) = \mu/[1 + \ln(\varepsilon_F/\varepsilon_{max})] \tag{6.5}$$

The same values for μ^* have been used in our T_c calculations (column 4 of table 1). The results clearly show that the cut-off $\varepsilon_{max} \simeq 50\omega_{Debye}$ is sufficiently high.

Our T_c values, T_c^{phon}, based on the phonon mechanism alone (column 3 of table 1) corroborate the results of previous calculations (Glötzel *et al* 1979): T_c^{phon} is near 20 K and lies far above experiment ($T_c^{exp} = 5.4$ K). As column 4 of table 1 shows, the spin fluctuations reduce T_c by as much as roughly a factor of 2. One might wonder why their influence on T_c is so sizeable though their contribution to the electronic mass enhancement is relatively small. The cause of this is that the spin fluctuations enter the anomalous self-energy in a different way from the normal self-energy. This can be seen by considering the following quantity, g:

$$g = (\beta/\pi)|\operatorname{Im}[\varepsilon_m + \tilde{\Sigma}(\varepsilon_m)]|\,|\tilde{K}^{sp}(\varepsilon_0, \varepsilon_0)|. \tag{6.6}$$

The quantity g may be considered as a measure for the strength of $\tilde{K}^{sp}$. In the case of V we obtain $g = 0.225$, a value that is considerably higher than the spin fluctuation mass enhancement. The corresponding quantity, g^{phon}, on the other hand, is identical to the mass enhancement due to the electron–phonon coupling mechanism.

7. Summary

We presented a theory for the superconducting transition temperature of transition metals in the frame of the local density functional theory and the RPA, and applied it to V. Its ingredients are the electronic structure, the phonon and spin fluctuation spectra and their coupling to the electrons. Except for the shell model parameters of the phonon spectrum, these quantities contain no adjustable parameters, thus superseding previous work (Rietschel and Winter 1979) employing jellium-like models. Furthermore we discussed numerical methods for setting up and solving the Eliashberg equations in the case of a crystalline lattice. In qualitative agreement with previous work (Rapp and Craford 1974, Rietschel and Winter 1979) we showed that spin fluctuations are able—at least within the LDA-RPA approximation—to lead to a considerable depression of T_c as compared with the number due to the pure phonon mechanism. We gave an argument as to why this can happen in spite of the low value of the spin fluctuation mass enhancement.

In spite of this significant effect the calculated T_c is still appreciably higher than the measured one. In this connection it is interesting to note that the T_c calculations of Glötzel *et al* (1979) for Nb, using $\mu^* = 0.13$, overestimate the experimental number for this substance as well. In our opinion these findings suggest that in neither V nor Nb is the effect of the spin-independent part of the Coulomb interaction on T_c adequately accounted for by such a small value for μ^* as proposed by McMillan (1968). To investigate this point further we intend to treat the density–density correlations and their coupling to the electrons within the RPA-LDA in future work and to implement them to the Eliashberg equations. It remains to be seen whether this can lead to a systematic description of the trends in the superconducting transition temperatures of transition metals.

Appendix 1

The local angular momentum representation of a Bloch state, $\Psi_{k\nu}(\boldsymbol{\rho})$ reads in the framework of the KKR band-structure method:

$$\Psi_{k\nu}(\boldsymbol{\rho}) = \sum_{l,m} c^{(k)}_{lm;\nu} Y_{lm}(\boldsymbol{\rho}) R_l(\rho, \varepsilon_{k\nu}). \tag{A1.1}$$

The c are the Bloch state coefficients, the Y_{lm} are the real spherical harmonics and the R_l are the energy-dependent radial parts of the single-site eigenstates in the muffin-tin potential.

Using the Kramers–Kronig relation the spin fluctuation propagator, $\chi^{s}_{q}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n - \varepsilon_m)$, of equation (2.2) may be written in the following form:

$$\chi^{s}_{q}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \varepsilon_n - \varepsilon_m) = \frac{2}{\pi} \int_0^\infty \mathrm{d}\omega' \, \frac{\omega'}{\omega'^2 - (\varepsilon_n - \varepsilon_m)^2} \operatorname{Im} \chi^{s}_{q}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \omega'). \tag{A1.2}$$

For $\chi^{s}_{q}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \omega)$ the following representation has been derived by Stenzel and Winter (1985):

$$\chi^{s}_{q}(\boldsymbol{\rho}, \boldsymbol{\rho}'; \omega) = \sum_{\substack{l,m,l',m',\\ l_1,\kappa_1,l_2,\kappa_2,\\ l'_1,\kappa'_1,l'_2,\kappa'_2}} Y_{lm}(\boldsymbol{\rho}) \tilde{R}_{l_1\kappa_1}(\rho) \tilde{R}_{l_2\kappa_2}(\rho)$$

$$\hat{\chi}_{q\omega}(lml_1\kappa_1 l_2\kappa_2 | l'm'l'_1\kappa'_1 l'_2\kappa'_2) Y_{l'm'}(\boldsymbol{\rho}') \tilde{R}_{l'_1\kappa'_1}(\rho') \tilde{R}_{l'_2\kappa'_2}(\rho'). \tag{A1.3}$$

For the definition of $\hat{\chi}$ see Stenzel and Winter (1985) and Stenzel *et al* (1988). The $\tilde{R}_{l\kappa}$ are the radial coordinate-dependent energy expansion coefficients of R_l, defined through the relation

$$R_l(\rho, \varepsilon) = \sum_{\kappa=1}^{\infty} \tilde{R}_{l\kappa}(\rho) \varepsilon^{\kappa-1}. \tag{A1.4}$$

The sum over κ has been truncated at $\kappa = 2$ for $l = 0, 1$ and at $\kappa = 3$ for $l = 2$. Inserting equations (A1.1) to (A1.4) into equation (2.6) we obtain

$$\begin{aligned} M^{s*}(\boldsymbol{q}\nu, \boldsymbol{k}\bar{\nu}) &\times \chi^{s}_{q-k}(\varepsilon_m - \varepsilon_n) \times M^{s}(\boldsymbol{k}\bar{\nu}, \boldsymbol{q}\nu) \\ &= \sum_{\substack{l,m,l',m',\\ l_1,m_1,l_2,m_2,l'_1,m'_1,l'_2,m'_2,\\ l_3,\kappa_3,l_4,\kappa_4,l'_3,\kappa'_3,l'_4,\kappa'_4}} G(lm, l_1m_1, l_2m_2) G(l'm', l'_1m'_1, l'_2m'_2) \\ &\times c^{*(q)}_{l_1m_1\nu} c^{(k)}_{l_2m_2\bar{\nu}} c^{*(k)}_{l'_2m'_2\bar{\nu}} c^{(q)}_{l'_1m'_1\nu} \\ &\times \int \rho^2 \, \mathrm{d}\rho \, R_{l_1}(\rho, \varepsilon_{q\nu}) R_{l_2}(\rho, \varepsilon_{k\bar{\nu}}) K^{s}_{xc}(\rho) \tilde{R}_{l_3\kappa_3}(\rho) \tilde{R}_{l_4\kappa_4}(\rho) \\ &\times \int \rho'^2 \, \mathrm{d}\rho' \, R_{l'_1}(\rho', \varepsilon_{q\nu}) R_{l'_2}(\rho', \varepsilon_{k\bar{\nu}}) K^{s}_{xc}(\rho') \tilde{R}_{l'_3\kappa'_2}(\rho') \tilde{R}_{l'_4\kappa'_4}(\rho') \\ &\times \frac{2}{\pi} \int_0^\infty \mathrm{d}\omega' \, \frac{\omega'}{\omega'^2 - (\varepsilon_n - \varepsilon_m)^2} \chi_{q-k,\omega}(lml_3\kappa_3 l_4\kappa_4 | l'm'l'_3\kappa'_3 l'_4\kappa'_4). \end{aligned} \tag{A1.5}$$

Here, the G are the Gaunt coefficients with respect to real spherical harmonics.

Appendix 2

With the help of the Bloch states representation (equation (A1.1)) it is straightforward to cast the expression for the phonon Eliashberg function (equation (2.12)) into a form amenable to numerical treatment. It reads

$$\alpha^2F(\omega) = \frac{1}{2Mn(\varepsilon_F)} \sum_{\substack{l_1,m_1,l_2,m_2,\\ l_1',m_1',l_2',m_2'}} \sum_{\nu_1,\nu_2,\lambda} \int \frac{d\boldsymbol{q}}{\Omega_{BZ}} \int \frac{d\boldsymbol{k}}{\Omega_{BZ}} \delta(\varepsilon_F - \varepsilon_{\boldsymbol{q}\nu_1})\delta(\varepsilon_F - \varepsilon_{\boldsymbol{q}\nu_2})$$

$$\times \frac{\delta(\omega - \omega_{\boldsymbol{q}-\boldsymbol{k},\lambda})}{\omega} c^{*(q)}_{l_1m_1,\nu_1} c^{(k)}_{l_2m_2,\nu_2} c^{(q)}_{l_1'm_1',\nu_1} c^{*(k)}_{l_2'm_2',\nu_2} (4\pi/3)^2$$

$$\times Y_1^m(\boldsymbol{e}_{\boldsymbol{q}-\boldsymbol{k},\lambda}) Y_1^{m'}(\boldsymbol{e}_{\boldsymbol{q}-\boldsymbol{k},\lambda}) G(lm, l_1m_1, l_2m_2) G(1m', l_1'm_1', l_2'm_2')$$

$$\times \{\sin[\delta_{l_1}(\varepsilon_F) - \delta_{l_1+1}(\varepsilon_F)]\Delta_{l_2,l_1+1} + \sin[\delta_{l_2}(\varepsilon_F) - \delta_{l_2+1}(\varepsilon_F)]\Delta_{l_1,l_2+1}\}$$

$$\times \{\sin[\delta_{l_1'}(\varepsilon_F) - \delta_{l_1'+1}(\varepsilon_F)]\Delta_{l_2',l_1'+1} + \sin[\delta_{l_2'}(\varepsilon_F) - \delta_{l_2'+1}(\varepsilon_F)]\Delta_{l_1',l_2'+1}\}$$

$$\times (N_{l_1}N_{l_2}N_{l_1'}N_{l_3'})^{-1}. \tag{A2.1}$$

Here, use has been made of the relation between the matrix elements of the gradient of the muffin-tin potential between the wavefunctions $R_l(\rho, \varepsilon_F)$ and the phase shifts $\delta_l(\varepsilon_F)$ (Gaspari and Gyorffy 1972). The normalisation factors are defined in the following way:

$$N_l = [j_l(\sqrt{\varepsilon_F}r_{mt}) \cos \delta_l(\varepsilon_F) - n_l(\sqrt{\varepsilon_F}r_{mt}) \sin \delta_l(\varepsilon_F)]/R_l(r_{mt}, \varepsilon_F) \tag{A2.2}$$

with $j_l(n_l)$ the spherical Bessel (Neumann) functions and r_{mt} the muffin-tin radius.

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