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SCATTERING PROPERTIES OF A NEAREST NEIGHBOUR CLUSTER

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I. Introduction

To investigate the influence of a substitutional impurity in a dilute alloy on the electronic structure and on the transport properties the perturbation of the crystal potential by the impurity must be known. Using the muffin-tin approximation of the crystal potential a first approximation includes a spherical perturbation within the muffin-tin sphere at the impurity site only. But there are perturbations at the neighbouring sites, too, arising from the extension of the wave functions of the impurity valence electrons into neighbouring Wigner-Seitz cells. Therefore a second approximation includes spherical perturbations at the first neighbour sites, too.

In the second approximation the whole perturbation is not a spherical one. That means the perturbed cluster around the impurity has anisotropic scattering properties not occuring in the first approximation. For the most symmetric case, twelve fcc nearest neighbours, the extend of that anisotropy is investigated by means of the method of generalized phase shifts for a cluster of muffin-tin potentials /1,2/ . According to this method the scattering behaviour of a cluster is characterized completely by the generalized phase shifts η_λ and an orthogonal and normalized set of partial wave amplitudes $A_\lambda(\vec{n}_r)$, which are found by calculating solutions of the Schrödinger equation for the energy $E = \kappa^2$ with the asymptotic behaviour

$$\phi_\lambda(\vec{r} \to \infty) = A_\lambda(\vec{n}_r) \frac{e^{i(\kappa r + \eta_\lambda)}}{2 i \kappa r} + c.c., \qquad \vec{n}_r \equiv \frac{\vec{r}}{r} . \tag{I.1}$$

The phase shifts result as eigenvalues of the set of homogeneous linear equations

$$\sum_{i',L'} [\delta_{ii'} \delta_{LL'} ctg\, \eta^{i}_{L} + N^{ii'}_{LL'} - ctg\, \eta_{\lambda} J^{ii'}_{LL'}] A^{i'}_{L'\lambda} = 0 \tag{I.2}$$

for the coefficients $A^{i}_{L\lambda}$, which characterize the wave function near the muffin-tins. The indices i and i' run over the different muffin-tin sites, L and L' over those angular momenta for which the phase shift of a single muffin-tin, η^{i}_{L}, is different from zero. $N^{ii'}_{LL'}$, and $J^{ii'}_{LL'}$, are characterized by the sites $\vec{R}_i$ of the muffin-tin potentials. After solving (I.2) the partial wave amplitudes can be calculated by

$$A_{\lambda}(\vec{n}_r) = \sum_{i,L} (-i)^{\ell} e^{-i\kappa \vec{n}_r \vec{R}_i} Y_L(\vec{n}_r) A^{i}_{L\lambda} . \tag{I.3}$$

2. *Nearest Neighbour Cluster*

In the fcc nearest neighbour cluster the muffin-tins are situated according to Fig.I. All sites have equal distance $R = |\vec{R}_i|$ from the origin. There are four distances between different sites: $R_{1i} = R$ for $i = 5,6, 11, 12$, $R_{1i} = \sqrt{2}\, R$ for $i = 2,4$, $R_{11} = \sqrt{3} R$ for $i = 7,8,9, 10$ and $R_{13} = 2R$. The phase shifts of the single muffin-tins are equal to each other in the problem considered here.

The evaluation is done for the simple case, that only the s-phase shift is different from zero, $\eta^{i}_{0} = \eta$. In this case only twelve coefficients $A^{i}_{0\lambda}$ appear in equation (I.2). They can be determined considering the cubic symmetry of the cluster, because the partial wave amplitudes $A_{\lambda}(\vec{n}_r)$ have to be irreducible representations of the corresponding symmetry group O_h . The absolute value of $A^{i}_{0\lambda}$ is given by the normalization condition $\int d\Omega\, |A_{\lambda}(\vec{n})|^2 = 1$. The realized representations λ are listed in Table I.

Table I
Realized irreducible representations

λ \ i	1	2	3	4	5	6	7	8	9	10	11	12		
1	+	+	+	+	+	+	+	+	+	+	+	+	Γ_1	monopole S
2	+	+	−	−	o	o	o	o	−	−	+	+	Γ_{15}	dipole P
3	+	−	−	+	+	+	−	−	o	o	o	o		
4	o	o	o	o	+	−	−	+	+	−	−	+		
5	+	+	+	+	−	−	−	−	o	o	o	o	Γ_{12}	quadrupole D
6	+	+	+	+	o	o	o	o	−	−	−	−		
7	+	−	+	−	o	o	o	o	o	o	o	o	Γ_{25}'	
8	o	o	o	o	+	−	+	−	o	o	o	o		
9	o	o	o	o	o	o	o	o	+	−	+	−		
10	+	+	−	−	o	o	o	o	+	+	−	−	Γ_{25}	octupole F
11	+	−	−	+	−	−	+	+	o	o	o	o		
12	o	o	o	o	+	−	−	+	−	+	+	−		

Expanding the exponential function of eq. (1.3) similar as in eq. (3.8) into cubic harmonics $Y_{\lambda'}(\vec n_r)$ the partial wave amplitudes $A_\lambda(\vec n_r)$ result next to as a sum of all cubic harmonics

$$A_\lambda(\vec n_r)=\sqrt{4\pi}\sum_\ell (-i)^\ell\, j_\ell(\kappa R)\sum_{\lambda'} Y_{\lambda'}(\vec n_r)\sum_i Y_{\lambda'}(\vec n_i)\, A^i_{0\lambda} \ . \tag{2.1}$$

But with

$$\sum_i Y_{\lambda'}(\vec n_i)\, A^i_{0\lambda}=\delta_{\lambda'\lambda} A_\lambda \ , \tag{2.2}$$

which guarantees as a consequence of Table I the amplitudes $A_\lambda(\vec n_r)$ to be really irreducible representations of O_h, only those angular momenta ℓ_λ contribute, which belong to the representation λ. Therefore the normalized amplitudes take the form

$$A_\lambda(\vec n_r)=\frac{\sum_{\ell_\lambda} (-i)^{\ell_\lambda}\, j_{\ell_\lambda}(\kappa R)\, Y_\lambda(\vec n_r)}{\sqrt{\sum_{\ell_\lambda} j^2_{\ell_\lambda}(\kappa R)}} \ . \tag{2.3}$$

If one takes into account only contributions up to $\ell = 2$, then according to the angular momentum expansion of the irreducible representations eq. (2.3) simplifies to

$$A_\lambda(\vec{n}_r) = (-i)^{\ell_\lambda} \, Y_\lambda(\vec{n}_r) \qquad \text{for} \quad \lambda = 1,\ldots,9. \tag{2.4}$$

The Γ'_{25} representation $\lambda = 10,11,12$ has no parts $\ell \leq 2$. The normalization factor of (2.3) is also approximated, so that the $A_\lambda(\vec{n}_r)$ of (2.4) are again normalized to l. According to the realized irreducible representations (Table I) each of the representations occurs only one time. Using the connection between the coefficients $A^i_{0\lambda}$ (Table I) equation (I.2) leads to a linear equation for each of the four different eigenvalues η_1, η_{15}, η_{12} and η'_{25}:

$$ctg\,\eta_1 = \frac{ctg\,\eta + 4n_0(\kappa R) + 2n_0(\sqrt{2}\,\kappa R) + 4n_0(\sqrt{3}\,\kappa R) + n_0(2\kappa R)}{1 + 4j_0(\kappa R) + 2j_0(\sqrt{2}\,\kappa R) + 4j_0(\sqrt{3}\,\kappa R) + j_0(2\kappa R)},$$

$$ctg\,\eta_{15} = \frac{ctg\,\eta + 2n_0(\kappa R) - 2n_0(\sqrt{3}\,\kappa R) - n_0(2\kappa R)}{1 + 2j_0(\kappa R) - 2j_0(\sqrt{3}\,\kappa R) - j_0(2\kappa R)},$$

$$ctg\,\eta_{12} = \frac{ctg\,\eta - 2n_0(\kappa R) + 2n_0(\sqrt{2}\,\kappa R) - 2n_0(\sqrt{3}\,\kappa R) + n_0(2\kappa R)}{1 - 2j_0(\kappa R) + 2j_0(\sqrt{2}\,\kappa R) - 2j_0(\sqrt{3}\,\kappa R) + j_0(2\kappa R)}, \tag{2.5}$$

$$ctg\,\eta'_{25} = \frac{ctg\,\eta - 2n_0(\sqrt{2}\,\kappa R) + n_0(2\kappa R)}{1 - 2j_0(\sqrt{2}\,\kappa R) + j_0(2\kappa R)}.$$

For low energies, as expected, $\eta_1 \sim \kappa$, $\eta_{15} \sim \kappa^3$ and $\eta_{12}, \eta'_{25} \sim \kappa^5$ holds, expressing the monopole-, dipole- and quadrupole-character, respectively, of the corresponding scattering states.

3. Scattering of a Plane Wave

The usual situation of scattering theory (incoming plane wave and outgoing spherical wave) is obtained by an appropriate linear combination /1/ :

$$\phi_{k}(\vec{r}) = 4\pi \sum_{\lambda} \phi_{\lambda}(\vec{r}) e^{i\eta_{\lambda}} A^{*}_{\lambda}(n_{k}), \quad \vec{n}_{k} \equiv \frac{\vec{k}}{k}, \quad k = \kappa . \tag{3.1}$$

Indeed, with the asymptotic behaviour (1.1) and with the completeness of the partial wave amplitudes

$$\sum_{\lambda} A_{\lambda}(\vec{n}_{r}) A^{*}_{\lambda}(\vec{n}_{k}) = \delta(\vec{n}_{r} - \vec{n}_{k}), \quad \vec{n}_{r} \equiv \frac{\vec{r}}{r} \tag{3.2}$$

from (3.1) follows

$$\phi_{\vec{k}}(\vec{r}) \to e^{i\vec{k}\vec{r}} + f(\vec{n}_{r}, \vec{n}_{k}) \frac{e^{ikr}}{r} \quad \text{for } r \to \infty \tag{3.3}$$

with the scattering amplitude /1/ ,

$$f(\vec{n}_{r}, \vec{n}_{k}) = \frac{4\pi}{\kappa} \sum_{\lambda} A_{\lambda}(\vec{n}_{r}) \sin\eta_{\lambda} e^{i\eta_{\lambda}} A^{*}_{\lambda}(\vec{n}_{k}) . \tag{3.4}$$

(3.4) shows, that the scattering states determined by the cluster equations (1.2) are simultaneously eigenstates of the scattering amplitude

$$\int d\Omega' \, f(\vec{n}, \vec{n}') A_{\lambda}(\vec{n}') = \frac{4\pi}{\kappa} \sin\eta_{\lambda} e^{i\eta_{\lambda}} A_{\lambda}(\vec{n}), \tag{3.5}$$

owing to the orthogonality of the partial wave amplitudes

$$\int d\Omega\, A^*_\lambda(\vec{n}) A_{\lambda'}(\vec{n}) = \delta_{\lambda\lambda'} \, . \tag{3.6}$$

Deriving (3.3), the formula

$$e^{i\vec{k}\vec{r}} \to \frac{4\pi}{2i\kappa r}\left[\delta(\vec{n}_r - \vec{n}_k)\, e^{ikr} - \delta(\vec{n}_r + \vec{n}_k)\, e^{-ikr}\right] \tag{3.7}$$

has been used, which follows from the expansion of a plane wave into spherical harmonics

$$e^{i\vec{k}\vec{r}} = 4\pi \sum_L i^\ell\, j_\ell(\kappa r) Y_L(\vec{n}_r) Y_L(\vec{n}_k) \tag{3.8}$$

and from the asymptotic behaviour of the spherical Bessel functions

$$j_\ell(\kappa r) \to \frac{\sin(\kappa r - \frac{\ell\pi}{2})}{\kappa r} \qquad \text{for} \quad r \to \infty \, . \tag{3.9}$$

4. Calculations of the Scattering Amplitude and Discussion

According to (3.4) the scattering amplitude $f(\vec{n}_r, \vec{n}_k)$ can be calculated from the generalized phase shifts η_λ and the partial wave amplitudes $A_\lambda(\vec{n}_r)$, determined in Section 2. For low energies (considering $\ell \lesssim 2$ only) the result is with the notation $\zeta = \vec{n}_r \vec{n}_k$

$$\begin{aligned} f(\vec{n}_r, \vec{n}_k) = \frac{1}{\kappa}\{ & e^{i\eta_1} \sin\eta_1 + 3 e^{i\eta_{15}} \sin\eta_{15} P_1(\zeta) \\ & + \frac{5}{2}(e^{i\eta_{12}} \sin\eta_{12} + e^{i\eta'_{25}} \sin\eta'_{25}) P_2(\zeta) \\ & + \frac{4\pi}{2}(e^{i\eta_{12}} \sin\eta_{12} - e^{i\eta'_{25}} \sin\eta'_{25}) \times [Y_{2+}(\vec{n}_r) Y_{2+}(\vec{n}_k) + \end{aligned} \tag{4.1}$$

$$+Y_{2-}(\vec{n}_r)Y_{2-}(\vec{n}_k)-Y_{2x}(\vec{n}_r)Y_{2x}(\vec{n}_k)-Y_{2y}(\vec{n}_r)Y_{2y}(\vec{n}_k)$$
$$-Y_{2z}(\vec{n}_r)Y_{2z}(\vec{n}_k)]\}. \tag{4.1}$$

Y_{2+}, Y_{2-} and Y_{2x}, Y_{2y}, Y_{2z} are the Γ_{12} and Γ'_{25} representations, respectively, of the $\ell=2$ spherical harmonics.

Equation (4.1) shows that the $\ell=0$ and $\ell=1$ part of $f(\vec{n}_r,\vec{n}_k)$ have an angular dependence equal to that of a spherical scatterer. The $\ell=2$ part differs according to the fact that the spherical harmonics combine to two different cubic representations Γ_{12} and Γ'_{25}.

Considering different wave vectors of the plane wave, $\vec{k}$, we find a different angular behaviour and different absolute values of $f(\vec{n}_r,\vec{n}_k)$. For $\vec{k}=\kappa(1,0,0)$, $\vec{k}=\frac{\kappa}{\sqrt{2}}(1,1,0)$ and $\vec{k}=\frac{\kappa}{\sqrt{3}}(1,1,1)$, respectively, we find for the $\ell=2$ part of $f(\vec{n}_r,\vec{n}_k)$:

$$f_2(\vec{n}_r;1,0,0)=\frac{5}{\kappa}(2e^{i\eta_{12}}\sin\eta_{12}-e^{i\eta'_{25}}\sin\eta'_{25})P_2(\zeta),$$

$$f_2(\vec{n}_r,1,1,0)=\frac{5}{\kappa}[e^{i\eta_{12}}\sin\eta_{12}P_2(\zeta)-(e^{i\eta_{12}}\sin\eta_{12}-e^{i\eta'_{25}}\sin\eta'_{25})\frac{3}{2}\frac{xy}{r^2}]. \tag{4.2}$$

$$f_2(\vec{n}_r;1,1,1)=\frac{5}{\kappa}e^{i\eta'_{25}}\sin\eta'_{25}P_2(\zeta).$$

We see that for an incoming plane wave in the $(1,0,0)$ or $(1,1,1)$ direction the angular behaviour of the scattered wave is equal to that of a spherical scatterer, for $\ell=2$, too. But the value of the amplitude is different for both directions. The difference is characterized by the amount of $\eta_{12}-\eta'_{25}$. For an incoming plane wave in the $(1,1,0)$ direction an angular dependence not only characterized by the angle ζ between $\vec{n}_r$ and $\vec{n}_k$ occurs.

For low energy the difference between η_{12} and η'_{25} can be calculated using (2.5):

$$\eta_{12}=\frac{(\kappa R)^5}{30(\frac{\kappa R}{\eta}+\frac{2}{\sqrt{2}}-\frac{3}{2}-\frac{2}{\sqrt{3}})},\quad \eta'_{25}=\frac{(\kappa R)^5}{15(\frac{\kappa R}{\eta}+\frac{1}{2}\pm\sqrt{2})}. \tag{4.3}$$

A numerical estimation leads to $\eta'_{25}/\eta_{12} \sim 2$ in the range $|\eta/\kappa R| < 1$, showing that the $\ell = 2$ part of the scattering amplitude can show a change of 100% comparing different wave vectors $\vec{k}$ and equal scattering angle ζ.

The results of these investigations show, that in simple metals where the wave functions of the valence electrons contain $s-$ and $p-$ parts mainly an impurity may be considered as a spherical perturbation. However in transition metals with d-electrons in the conduction band the perturbation at nearest neighbour sites must be taken into account to explain the anisotropy of transport properties exactly.

The investigations given here can be extended to higher angular momenta and to muffin-tins with p-and d-phase shifts different from zero on the same line in a streightforward way.

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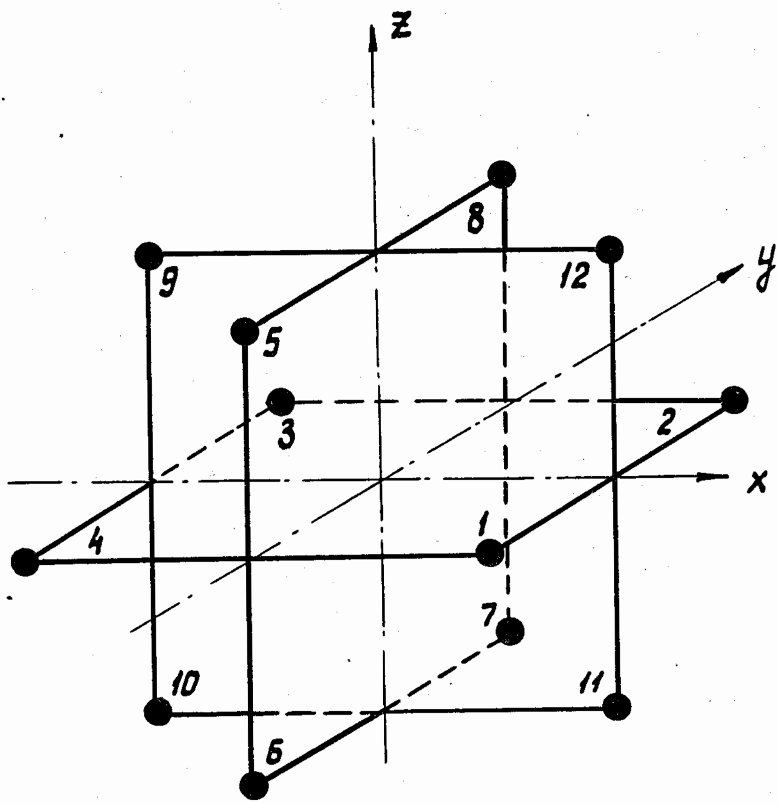

Fig. 1. Twelve nearest neighbour cluster.