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**THE ELECTRON-PHONON MASS
ENHANCEMENT IN TRANSITION METALS**

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**ЛАБОРАТОРИЯ
ТЕОРЕТИЧЕСКОЙ ФИЗИКИ**

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**THE ELECTRON-PHONON MASS
ENHANCEMENT IN TRANSITION METALS**

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Recently Gaspari and Gyorffy (1972, to be referred to as 1) have developed a theory for the calculation of the electron-phonon mass enhancement λ in transition metals (see also Stocks et al. 1972 and Evans et al. 1973). Their results show, that the electronic contribution to λ is dominated by the scattering properties of the atomic potential. This circumstance allows an estimation of λ from the scattering phase shifts of the atomic potential without a full band-structure calculation. However in order to obtain these results the authors assume that the energy bands are spherical. The main concern of this letter is to show that this approximation - which is at first sight a severe approximation - is unnecessary. An exact evaluation gives - at least for cubic crystals - the same expression for λ as in 1 with an insignificant redefinition of some quantities.

Let us start as in 1 with the electron-phonon mass enhancement factor λ given by McMillan (1968)

$$\lambda = \frac{D(E_F) \langle I^2 \rangle}{M \langle \omega^2 \rangle} \quad (1)$$

where $D(E_F)$ is the spin density of states per atom at the Fermi energy E_F , $\langle \omega^2 \rangle$ is an average of the square of the phonon frequency and M is the atomic mass. The averaged electron-phonon matrix element $\langle I^2 \rangle$ can be written - instead of expressing it as in 1 by Bloch states - by means of the retarded Green function $G(\vec{r}, \vec{r}; E)$

$$\langle I^2 \rangle = \frac{1}{\pi^2 D^2(E_F)} \iint d\vec{r} d\vec{r}' \nabla v(\vec{r}) \nabla' v(\vec{r}') \{ \text{Im} G(\vec{r}, \vec{r}', E_F) \}^2 \quad (2)$$

Note that we use units where $\hbar = 2m = 1$.

We make use of an expression for the Green function given by Gyorffy and Stott (1971) (see also Lloyd and Smith 1972, Lehmann 1973). If \vec{r} and \vec{r}' are both inside the muffin-tin radius r_m the imaginary part of the Green function may be written in the form:

$$\text{Im} G(\vec{r}, \vec{r}', E) = -\kappa \sum_{L, L'} A_{LL'} J_L(\vec{r}) J_{L'}(\vec{r}'), \quad \kappa = \sqrt{E}, \quad (3)$$

where $J_L(\vec{r})$ is the regular solution of the Schrödinger equation for a single muffin-tin potential normalized so that

$$J_L(\vec{r}) = \{ \cos \eta_\ell j_\ell(\kappa r) - \sin \eta_\ell n_\ell(\kappa r) \} Y_L(\vec{r}) \quad (4)$$

for $r > r_m$. j_ℓ and n_ℓ are the spherical Bessel and Neumann functions. The Y_L are real spherical harmonics. L denotes the quantum numbers of the angular momentum ℓ and m . The muffin tin potential is characterized by the scattering phase shifts η_ℓ . The matrix $A_{LL'}$ only depends on the phase shifts η_ℓ and the crystal structure via the KKR structure constants (Lehmann 1973). The matrix $A_{LL'}$ may be expressed by the scattering path operator $T_{LL'}^{nn'}$ introduced by Gyorffy and Stott (1971)

$$A_{LL'} = (\kappa \sin \eta_\ell \sin \eta_{\ell'})^{-1} \text{Im} T_{LL'}^{nn'} \quad (5)$$

or by the generalized phase shifts η_λ (John and Ziesche 1971)

$$A_{LL'} = \sum_{\lambda} a_{L\lambda}^n a_{L'\lambda}^{n'} \sin^2 \eta_\lambda \quad (6)$$

For the diagonal elements A_{LL} immediately follows from equation (3) the relation

$$A_{LL} = \frac{d_L}{d_L^{(1)}}, \quad (7)$$

where d_L is the L component of the density of states within the muffin tin sphere in the crystal and $d_L^{(1)}$ the corresponding density of states in the case of a single scatterer:

$$d_L^{(1)} = \frac{\kappa}{\pi} \int_{r < r_m} d\vec{r} J_L^2(\vec{r}). \quad (8)$$

Substituting equation (3) in equation (2) and performing the integration over the muffin tin sphere gives an expression which only involves the scattering phase shifts and the coefficients $A_{LL'}$. Let us restrict our consideration to the important case of a cubic crystal with only non-zero phase shifts η_ℓ ($\ell=0,1,2$). Using cubic harmonics the matrix $A_{LL'}$ is diagonal with four independent coefficients only, corresponding to the irreducible representations Γ_1 ($\ell=0$), Γ_{15} ($\ell=1$), and Γ'_{25} , Γ'_{12} ($\ell=2$). In this case we immediately obtain from equation (2) the exact result:

$$D(E_F) \langle I^2 \rangle = \frac{E_F}{\pi^2 D(E_F)} \sum_{\ell=0}^2 2(\ell+1) \sin^2(\eta_{\ell+1} - \eta_\ell) \frac{d_{\ell+1} d_\ell}{d_{\ell+1}^{(1)} d_\ell^{(1)}}, \quad (9)$$

which is an expression very close to equation (7) in 1. In contrast to the results in 1 equation (9) involves the densities of states within the muffin tin sphere

$$d_\ell = \sum_{m=-L}^L d_L, \quad d_\ell^{(1)} = (2\ell+1) d_L^{(1)}, \quad (10)$$

instead of the densities within the Wigner-Seitz sphere. The fact, that the cubic symmetry produces different densities of states d_L for the irreducible representation Γ'_{25} and Γ'_{12} with the same angular momentum $\ell=2$, has no influence, as the equation (9) only depends on the sum d_ℓ of these two densities. Accordingly the equation (7) in 1 is a good approximation in cubic close packed structure. However for a crystal with a lower symmetry than the cubic one the full matrix $A_{LL'}$ must be taken into account and the equation (9) is not valid. In this case the spherical approximation neglects the nondiagonal elements $A_{LL'}$. However it seems likely that these nondiagonal elements are small in the case of weak s and p scattering. In addition in the spherical

approximation the diagonal elements A_{LL} are replaced by an average which depends on the angular momentum l . A suitable way to calculate in a direct manner the matrix $A_{LL'}$ is a cluster approach using equation (5) or (6). This cluster method - which takes into account multiple scattering only between a small number of atoms - has been successfully used for the calculation of the density of states in disordered systems (McGill and Klima 1970 and 1972, Keller 1971, Keller and Jones 1971, John 1973). Since the cluster method gives reasonable results even in the case of strong scattering, the matrix $A_{LL'}$ may be obtained by relatively small clusters for transition metals. By the way, the same matrix $A_{LL'}$ is needed in the theory of soft X-ray emission spectra (Gyorffy and Stott 1971) and in the theory of point defects (Lehmann 1973).

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References

- Evans R., Gaspari C.D. and Gyorffy B.L., 1973, *J. Phys. F*, 3, 39-54.
Gaspari G.D. and Gyorffy B.L., 1972, *Phys. Rev. Lett.*, 28, 801-05.
Gyorffy B.L. and Stott M.J., 1971, *Solid State Comm.*, 9, 613-17.
John W., 1973, *phys. stat. sol. (b)*, 55, 801-09.
John W. and Ziesche P., 1971, *phys. stat. sol. (b)*, 47, 555-64.
Keller J. 1971, *J. Phys. C*, 4, 3143-54.
Keller J. and Jones R., 1971, *J. Phys. F*, 1, L33-36.
Lehmann G., 1973, *phys. stat. sol. (b)*, to be published.
Llyod P. and Smith P.V., 1972, *Adv. Physics*, 21, 69-152.
McMillen W.L., 1968, *Phys. Rev.*, 167, 331-44.
McGill T.C. and Klima J., 1970, *J. Phys.*, C, 3, L163-67.
McGill T.C. and Klima J., 1972, *Phys. Rev.*, B5, 1517-28.
Stocks G.M., Gaspari G.D. and Gyorffy B.L., 1972, *J. Phys.*, F, 2, L123-28.

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