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ИНСТИТУТА  
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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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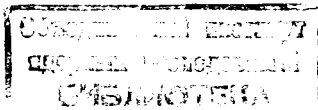
ON THE USE  
OF GENERALIZED PHASE SHIFTS  
IN SOLID STATE THEORY

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The scattering properties of spherically symmetric potentials are usually described by phase shifts  $\eta_\ell$ . To describe also the scattering properties of non-spherically symmetric potentials (molecules) Demkov and Rudakov /1/ recently introduced generalized phase shifts  $\eta_\lambda$  and corresponding partial wave amplitudes

$$A_\lambda(\vec{n}) = \sum_L (-i)^\ell Y_L(\vec{n}) A_{L\lambda}, \quad L \hat{=} (\ell, m_\ell), \quad \vec{n} = \frac{\vec{r}}{r}, \quad (1)$$

entering into the asymptotic behaviour of the scattering states as follows

$$\phi_\lambda(r \rightarrow \infty) \rightarrow A_\lambda(n) \frac{e^{i(\kappa r + \eta_\lambda)}}{2i\kappa r} + c.c., \quad \kappa = \sqrt{E}. \quad (2)$$

This concept is useful also in electron theory of solids for both ordered and disordered systems.

By means of such phase shifts  $\eta_\lambda$  and amplitudes  $A_{L\lambda}$  the Korringa-Kohn-Rostoker-scheme /2/ for band structure calculations can easily be generalized to non-spherically symmetric potentials within the (non-overlapping) muffin-tin spheres /3/ :

$$\det \left\| \sum_{L, L'} \tilde{A}_{\lambda L} i^{\ell-\ell'} B_{LL'}(\vec{k}) A_{L'\lambda} + \kappa \cot \eta_\lambda \delta_{\lambda\lambda} \right\| = 0. \quad (3)$$

The lattice structure is contained only in the usual *KKR*-structure matrices  $B_{LL'}(\vec{k})$ , while the *MT*-potential enters only via  $\eta_\lambda$  and  $A_{L\lambda}$ , determined by a coupled set of differential equations for the radial parts  $R_{L\lambda}(r)$  of the scattering wave functions  $\phi_\lambda(\vec{r})$ . This generalization (3) allows to overcome both restrictions of the usual *KKR*-method:

1. The assumption of constant potential between the MT-spheres is of course reasonable only for close-packed structures. But in the case of the more open structure of diamond type non-constant interstitial potential must be taken into account, for example by installation of additional MT-potentials at interstitial sites between the atoms. This has been done first by Keller /4/ using spherically symmetric potentials within the interstitial spheres. But these interstitial potentials are generally non-spherically symmetric. Such interstitial potentials increase of course the number of scatterers in the unit cell. Although the method for lattices with several atoms per unit cell already exists, it is useful to consider all scatterers in the unit cell as a whole and to describe the scattering properties of such clusters as in (3) by means of generalized phase shifts  $\eta_\lambda$  and amplitudes  $A_{L\lambda}$ .

2. The assumption of spherically symmetric MT-potentials at the atomic sites must be corrected, if for instance transition metals with partially filled d-bands /5/ or semiconductors with covalent bonds /6/ are considered. In this case (3) can also be applied.

In the case of a lattice with several atoms per unit cell (with phase shifts  $\eta_L^n$  at positions  $\vec{a}_n$ ), the corresponding cluster phase shifts  $\eta_\lambda$  are as recently shown by John and Ziesche /7/ determined by an algebraic eigenvalue equation

$$\sum_{n', L'} [ N_{LL'}^{nn'} - ctg \eta_\lambda J_{LL'}^{nn'} + ctg \eta_L^n \delta_{nn'} \delta_{LL'} ] A_{L'\lambda}^{n'} = 0. \quad (4)$$

$N_{LL'}^{nn'}$ , and  $J_{LL'}^{nn'}$  are certain matrices depending only on the cluster structure within the unit cell:

$$N_{LL'}^{nn'} = (1 - \delta_{nn'}) 4\pi \sum_{L''} C_{LL'L''} i^{l-l'+l''} n_{l''}(\kappa a_{nn'}) Y_{L''}(\frac{\vec{a}_{nn'}}{a_{nn'}}) \quad (5)$$

$$J_{LL'}^{nn'} = 4\pi \sum_{L''} C_{LL'L''} i^{l-l'+l''} j_{l''}(\kappa a_{nn'}) Y_{L''}(\frac{\vec{a}_{nn'}}{a_{nn'}}).$$

$$\vec{a}_{nn'} = \vec{a}_n - \vec{a}_{n'}$$

The amplitudes  $A_{L\lambda}$  follow via the solution of (4) from

$$A_{L\lambda} = \sum_{n', L'} J_{LL'}^{on'} A_{L'\lambda}^{n'}. \quad (6)$$

This approach is of interest for band calculations of lattices having complex unit cells with many atoms. The following advantages exist:

1. The eigenvalue problem (4) is independent of the Bloch vector.
2. The number of essentially non-zero cluster phase shifts increases only with the

linear dimension of the unit cell. This means, that some of the cluster phase shifts are very small for a given energy. This was shown by Demkov and Rudakov /1/ for the case of s-scatterers. The decrease of the number of phase shifts of course reduces also the dimension of the KKR matrices (3).

3. Variations of the atomic sites or potentials within the unit cell can easily be handled.

Besides this, by eliminating of  $\eta_{\lambda}$  and  $A_{L\lambda}$ , the KKR-equations for a lattice with base immediately follow in a form recently derived by Lehmann /8/ in a different manner:

$$\sum_{n', L'} \left[ \sum_{L''} i^{l-l''} B_{LL''}(\vec{k}) J_{L''L'}^{nn'} + \kappa N_{LL'}^{nn'} + \kappa \text{ctg} \eta_L^n \delta_{nn'} \delta_{LL'} \right] C_{L', \vec{k}}^{n'} = 0. \quad (7)$$

Here the structure matrices for the corresponding Bravais lattice and for the cluster forming the base appear in a factorized manner. From (3) now follows the physical background of this factorisation, because into (3) there enter only the structure of the Bravais lattice and the asymptotic scattering properties of the cluster, assumed the sites  $\vec{a}_n$  of its atoms are inside the incircled sphere of the unit cell.

Another possible application of generalized scattering states could be the following /9/: Introducing thin skins of zero potential along the unit cell surfaces, the whole crystal potential is split into a sum of non-overlapping, but generalized muffin-tin potentials, each non-zero within the whole unit cell. Assuming the scattering states of a single unit cell are known, again modified, but rather complicated KKR-equations can be derived containing unfortunately not only the asymptotic scattering properties, but also certain near field properties along the unit cell surfaces. The loss of the rigorous separation of the crystal structure and potential properties is connected with this fact.

Disordered systems are another field of application. For example the Lloyd - formula /10/ for the density of states can be very easily obtained from (4) via a generalized Friedel sum rule /11/. Using general properties of the generalized phase shifts new gap criteria for binary alloys can be derived /12/.

There are further possibilities for the application of generalized phase shifts. For example, the scattering properties of point defects, which are important in the theory of residual resistance, can be described by such phase shifts.

Finally, it can be concluded, that generalized scattering states are useful not only in the theory of molecules but also in the theory of solids.

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