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P. Ziesche

K-MATRICES AND T-MATRICES FOR FINITE SYSTEMS OF GENERAL MUFFIN-TIN POTENTIALS

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K-MATRICES AND T-MATRICES FOR FINITE SYSTEMS OF GENERAL MUFFIN-TIN POTENTIALS

* On leave from Technical University Dresden, GDR.

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Цише П.

K-матрицы и *T*-матрицы для конечных систем обобщенных потенциалов типа мафин-тин

Рассмотрены обобщенные потенциалы типа "мафин-тин", имеющие ненулевое значение в несферических областях произвольной формы и равные нулю вне ее, и их состояния рассеяния, причем, последние асимптотически описываются обобщенными фазами рассеяния и амплитудами парциальных волн. Диагональные по энергии *K*- и *T*-матрицы выражаются через эти асимптотические величины. Выведены *K*- и *T*-матрицы, диагональные по энергии, и их собственные состояния для некоторой произвольной совокупности обобщенных потенциалов типа "мафин-тин", окружающие сферы которых могут перекрываться. Полученные результаты обсуждаются.

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Ziesche P.

K-Matrices and *T*-Matrices for Finite Systems of General Muffin-Tin Potentials

General muffin-tin potentials, defined to be nonzero within arbitrary volumes and zero outside, and their scattering states, asymptotically described by generalized phase shifts and partial wave amplitudes, are considered. The *K*- and *T*-matrices on the energy shell are expressed by these asymptotic quantities. For a cluster of general muffin-tin potentials, the enveloping spheres of which may overlap, the *K*-and *T*- matrices on the energy shell and their eigenstates are derived and discussed.

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1. Introduction

The well-known concept of muffin-tin (MT) potentials, useful both in solid state theory and in the theory of molecules, has been generalized recently to clusters of MT-potentials [1,2] to finite sets of angular momenta coupling potentials [3,4] and more general to potentials being nonzero within arbitrary volumes [4], the enveloping spheres of which may overlap or not. Such generalized, non-spherically symmetric MT-potentials have several possibilities of application and aspects of usefulness as summarizing mentioned in [4]. The equations determining the (both scattering and bound) eigenstates ϕ_λ of such general MT-potentials have been derived in [2] and [4] using partially the ideas of the KKR-method. As mentioned in [5,6] these eigenstates ϕ_λ correspond to the eigenstates of the K-, T- or S -matrices of these potentials on the energy shell. In the following this correspondence will be treated in more detail. This makes more clear simultaneously the connection of [2] and [4] with the multiple scattering theory of Lloyd [7,8], Beeby [9] and Beeby and Edwards [10]. In this usual multiple scattering theory the spherically symmetric [8-10] or non-spherically symmetric [7] scatterers are assumed to be nonoverlapping spheres. Such a cluster is characterized by a K- (or T-) matrix involving only the scattering sites (centres of the spheres) and the asymptotic or far field properties of the single scattering potentials [7,11]. These far field properties of a singe scatterer are described by its K- (or T-) matrix on the energy shell. Here an attempt is started to treat also more general case of non-overlapping potentials within non-spherically symmetric volumes, the envelopping spheres of which may overlap. Such a more complicated cluster is characterized by a $K-$(or $T-$)matrix involving as above far field properties of the single scatterers, but generalized structure matrices instead of the usual ones. While the usual structure matrices contain really only the structure (that is, the scattering sites), in the generalized ones certain near field properties of the single scatterers occur. This reflects the fact, that the far fields are only valid outside the envelopping spheres. Therefore in the case of overlapping envelopping spheres these far fields are not sufficient, although the potential between the scattering regions is zero inplying there a free space behaviour. It is hoped, that the developped formalism is useful for generalizations of both the KKR method for bandstructure calculations of ordered MT-systems and Lloyd's formula for the density of states of disordered MT-systems.

In Section 1 a single general MT-potential is considered. The scattering amplitude and the $K-$and T -matrices on the energy shell are expressed by the generalized phase shifts and by the corresponding partial wave amplitudes. Two simple examples are discussed: A potential, coupling a finite set of angular momenta, and a cluster of usual (that is, spherically symmetric) MT-potentials. In Section 2 for a cluster of general MT's the $K-$and T -matrices on the energy shell are derived. Their eigenvalues determine the generalized phase shifts of the cluster and their eigenvectors are the corresponding partial wave amplitudes, entering into the expression for the wave functions. Also the trivial scattering states with vanishing phase shifts are included in the discussion. Subdividing such a cluster arbitrary into subclusters, then the multiple scattering within the whole cluster is fully taken into account, if the multiple scattering within and between these subclusters is fully taken into account.

2. A Single General MT-Potential

In /4/ the eigenstates of a general MT-potential, defined to be non-zero within an arbitrary volume V, have been discussed. In the far field region outside the envelopping sphere the scattering states are of the form (detonation see /4/)

$$\phi_\lambda(\vec{r}) = \sum_L [j_L(\vec{r}) A_{L\lambda} \cos\eta_\lambda - n_L(\vec{r}) A_{L\lambda} \sin\eta_\lambda] \text{ for } r > r_0. \quad (2.1)$$

Using Kasterin's representation of the spherical Bessel and Neumann functions (see for example /12/) these generalized MT-orbitals (2.1) can be rewritten as

$$\phi_\lambda(\vec{r}) = A_\lambda\left(\frac{\partial}{\kappa i \partial\vec{r}}\right)\frac{e^{i(\kappa r+\eta_\lambda)}}{2i\kappa r} + c.c. \quad \text{for } r > r_0. \quad (2.2)$$

with the partial wave amplitudes

$$A_\lambda(\vec{n}) \equiv \sum_L (-i)^\ell Y_L(\vec{n}) A_{L\lambda}. \quad (2.3)$$

Because the coefficients $A_{L\lambda}$ can be chosen real without loss in generality, the amplitudes have the property $A^*_\lambda(-\vec{n}) = A_\lambda(\vec{n})$. (2.1) shows clearly the asymptotic behaviour of a spherical wave with a certain linear combination of angular momenta, (2.3), incoming with a phase shift $-\eta_\lambda$ and outgoing with a phase shift $+\eta_\lambda$. The usual situation of scattering theory, namely an incoming plane wave and an outgoing spherical wave, is obtained from (2.2) by a certain linear combination (see /1/)

$$\phi_{\vec{\kappa}}(\vec{r}) = 4\pi \sum_\lambda \phi_\lambda(\vec{r}) e^{i\eta_\lambda} A^*_\lambda\left(-\frac{\vec{\kappa}}{\kappa}\right), \quad (2.4)$$

yielding really

$$\phi_{\vec{\kappa}}(\vec{r}) = e^{i\vec{\kappa}\vec{r}} + f\left(\frac{\partial}{i\kappa\partial\vec{r}}, \frac{\vec{\kappa}}{\kappa}\right)\frac{e^{i\kappa r}}{r} \quad (2.5)$$

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* This formula is very similar to an approach, recently discussed by R.Lenk, Karl-Marx-Stadt, GDR (private communication).

with a scattering amplitude

$$f(\vec{n},\vec{n}') = \frac{4\pi}{\kappa}\sum_{\lambda} A_{\lambda}(\vec{n}) \sin\eta_{\lambda}\, e^{i\eta_{\lambda}} A^{*}_{\lambda}(\vec{n}'). \qquad (2.6)$$

Deriving (2.5), the usual expansion of a plane wave into spherical harmonics

$$e^{i\vec{\kappa}\vec{r}} = 4\pi \sum_{L} i^{\ell} j_{L}(\vec{r}) Y_{L}\left(\frac{\vec{\kappa}}{\kappa}\right) = 4\pi \sum_{L} Y_{L}\left(\frac{\partial}{i\kappa\partial\vec{r}}\right) Y_{L}\left(\frac{\vec{\kappa}}{\kappa}\right) \frac{\sin\kappa r}{\kappa r} \qquad (2.7)$$

has been used.

The connection of (2.6) with the T-matrix, defined by

$$T = V + VG^{\circ}_{+} T, \quad G^{\circ}_{+}(\vec{r}-\vec{r}') \equiv -\frac{e^{i\kappa|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \qquad (2.8)$$

follows simple from its connection with the K-matrix defined by

$$K = V + VG^{\circ}K, \quad G^{\circ}(\vec{r}-\vec{r}') \equiv -\frac{\cos\kappa|\vec{r}-\vec{r}'|}{4\pi|\vec{r}-\vec{r}'|}. \qquad (2.9)$$

Namely as a consequence of these definitions, it holds

$$T = K(1 - iG^{\circ}_{h} K), \quad iG^{\circ}_{h} \equiv G^{\circ}_{+} - G^{\circ} \qquad (2.10)$$

with a homogeneous Green's function

$$G^{\circ}_{h}(\vec{r}-\vec{r}') = -\frac{\sin\kappa|\vec{r}-\vec{r}'|}{4\pi|\vec{r}-\vec{r}'|} = -\kappa\sum_{L} j_{L}(\vec{r}) j_{L}(\vec{r}'). \qquad (2.11)$$

With this expansion of G°_{h} the matrices on the energy shell $K_{LL'} \equiv (j_{L}, K j_{L'})$ and $T_{LL'} \equiv (j_{L}, T j_{L'})$ are connected with each other owing to (2.10) via

$$T_{LL'} = \sum_{L''} K_{LL''}[(1 + i\kappa K)^{-1}]_{L''L'}. \qquad (2.12)$$

As discussed in /4/ the coefficients $A_{L\lambda}$ form as eigenvectors of the hermitian matrix $K_{LL'}$ an orthogonal and complete set. Therefore $K_{LL'}$ can be written as

$$K_{LL'} = \sum_{\lambda} A_{L\lambda} K_{\lambda} \tilde{\tilde{A}}_{\lambda L'}, \quad K_{\lambda} = -\frac{1}{\kappa}\, tg\,\eta_{\lambda}. \qquad (2.13)$$

Inserting this into (2.12) yields

$$T_{LL'} = \sum_{\lambda} A_{L\lambda} T_{\lambda} \tilde{\tilde{A}}_{\lambda L'}, \quad T_{\lambda} = K_{\lambda}(1 + i\kappa K_{\lambda})^{-1} = -\frac{1}{\kappa} \sin\eta_{\lambda}\, e^{i\eta_{\lambda}}, \qquad (2.14)$$

showing that the coefficients $A_{L\lambda}$ are simultaneously eigenvectors of $T_{LL'}$ and that the scattering amplitude (2.6) differs from the T-matrix on the energy shell

$$\begin{aligned} T(\vec{n},\vec{n}') &= \int d\vec{r} \int d\vec{r}'\, e^{-i\kappa\vec{n}\vec{r}}\, T(\vec{r},\vec{r}')\, e^{i\kappa\vec{n}'\vec{r}'} \\ &= \sum_{L,L'} (i)^{\ell}\, Y_{L}(\vec{n})\, T_{LL'}\, i^{\ell'} Y_{L'}(\vec{n}') \\ &= \sum_{\lambda} A_{\lambda}(\vec{n})\, T_{\lambda}\, A_{\lambda}(\vec{n}') \end{aligned} \qquad (2.15)$$

only by a factor -4π. For completeness the wave function is expressed in terms of K- and T-matrix, respectively,

$$\begin{aligned} \phi_{\lambda} &= (1 + G^{\circ}K)\, j_{\lambda} \cos\eta_{\lambda}, \\ \phi_{\lambda} &= (1 + G^{\circ}_{+} T)\, j_{\lambda}\, e^{-i\eta_{\lambda}}, \end{aligned} \qquad j_{\lambda} \equiv \sum_{L} j_{L} A_{L\lambda}, \qquad (2.16)$$

involving matrix elements outside the envelopping sphere (far field) only on the energy shell, but inside (near field) also off the energy shell. Indeed with

$$G^{\circ}(\vec{r}-\vec{r}') = \kappa \sum_{L} n_{L}(\vec{r}) j_{L}(\vec{r}') \quad \text{for } r > r' \qquad (2.17)$$

one obtains for example

$$\phi_\lambda(\vec r) = j_\lambda(\vec r)\cos\eta_\lambda + \kappa \sum_{L,L'} n_L(\vec r) K_{LL'} A_{L'\lambda} \cos\eta_\lambda \quad \text{for } r > r_0 , \tag{2.18}$$

which agrees with (2.1) via (2.13).

Finally the K- and T-matrices are given for two simple examples of non-spherically symmetric MT-potentials. Also a generalized logarithmic derivative at $r = r_0$, defined by

$$D_{LL'} \equiv \sum_\lambda \frac{dR_{L\lambda}}{dr} (R^{-1})_{\lambda L'} \Big|_{r=r_0} \tag{2.19}$$

and occuring in the APW-method for such non-spherically symmetric MT-potentials /6/ will be given for completeness.

First we discuss a potential coupling a finite set of angular momenta $\ell \le \ell_0$. As discussed in /3/ and /4/ the Schrödinger equation yields $(\ell_0+1)^2$ solutions, the radial parts of which, R_{Ln} and its derivative R'_{Ln} at $r = r_0$ determine coefficients

$$a_{Ln} = \kappa r_0^2 [n'_\ell R_{Ln} - n_\ell R'_{Ln}]_{r=r_0} ,$$

$$\beta_{Ln} = \kappa r_0^2 [j'_\ell R_{Ln} - j_\ell R'_{Ln}]_{r=r_0} , \tag{2.20}$$

describing the wave function outside the envelopping sphere (see /4/ eq. (5.3)). Then the scattering states ϕ_λ are obtained by an appropriate linear combination $\sum_n \phi_n \gamma_{n\lambda}$, demanding

$$\sum_n a_{Ln}\gamma_{n\lambda} = A_{L\lambda}\cos\eta_\lambda , \quad \sum_n \beta_{Ln}\gamma_{n\lambda} = A_{L\lambda}\sin\eta_\lambda . \tag{2.21}$$

Instead of solving (2.21) and calculating the K-, and T- and D-matrices via (2.13), (2.14) and (2.19), respectively, these quantities can be evaluated directly from the coefficients (2.20) using the fact, that in this case the amplitudes $A_{L\lambda}$ of the $(\ell_0+1)^2$ non-trivial scattering states

form itself (that is, without the trivial scattering states) a complete set. Therefore from (2.21) follows

$$\sum_{n,\lambda} a_{Ln}\gamma_{n\lambda} \frac{1}{\cos\eta_\lambda} \overset{\approx}{A}_{\lambda L'} = \delta_{LL'} , \tag{2.22}$$

$$\sum_{n,\lambda} (a_{Ln} - i\beta_{Ln})\gamma_{n\lambda} e^{i\eta_\lambda} \overset{\approx}{A}_{\lambda L'} = \delta_{LL'} ,$$

yielding immediately the expressions

$$K_{LL'} = -\frac{1}{\kappa}\sum_n \beta_{Ln}(a^{-1})_{nL'} ;$$

$$T_{LL'} = -\frac{1}{\kappa}\sum_n \beta_{Ln}[(a - i\beta)^{-1}]_{nL'} ; \tag{2.23}$$

$$D_{LL'} = \sum (j'_\ell a_{Ln} - n'_\ell \beta_{Ln})[(ja - n\beta)^{-1}]_{nL'}\Big|_{r=r_0}$$

$D_{LL'}$ can be expressed even directly by the original quantities R_{Ln} and R'_{Ln}

$$D_{LL'} = \sum_n R_{Ln}(R^{-1})_{nL'}\Big|_{r=r_0} \tag{2.24}$$

owing to the Wronski-relation.

As a second simple example we consider a cluster of usual (spherically symmetric) MT-potential, characterized by sites $\vec R_i$ and phase shifts η^i_L. Again, instead of calculating the cluster phase shifts η_λ and amplitudes $A_{L\lambda}$ and inserting these results into (2.13), (2.14) and (2.19), the quantities of inserter can be expressed directly by $\vec R_i$ and $K^i_L = (-1/\kappa)\, tg\,\eta^i_L$:

$$K_{LL'} = \sum_{\substack{i_1,L_1\\ i_2,L_2}} J^{0 i_1}_{LL_1} (M^{-1})^{i_1 i_2}_{L_1 L_2} K^{i_2}_{L_2} J^{i_2 0}_{L_2 L'} ,$$

$$M^{ii'}_{LL'} \equiv \delta_{ii'}\delta_{LL'} - \kappa K^i_L N^{ii'}_{LL'} ,$$

$$T_{LL'} = \sum_{\substack{i_1,L_1\\ i_2,L_2}} J^{0 i_1}_{LL_1} (R^{-1})^{i_1 i_2}_{L_1 L_2} K^{i_2}_{L_2} J^{i_2 0}_{L_2 L'} ,$$

$$R^{ii'}_{LL'} = \delta_{ii'}\delta_{LL'} - \kappa K^i_L (N^{ii'}_{LL'} - iJ^{ii'}_{LL'}),$$

(2.25)

$$D_{LL'} = \sum_{L''} [j'_\ell \delta_{LL''} + n'_\ell \kappa K_{LL''}][(j + n\kappa K)^{-1}]_{L''L'}|_{r=r_0}.$$

The expressions for K and T are a special case of (3.8) and (3.28), derived in the following Section, and agree with the results of [7,8] and [11].

3. Clusters of General MT-Potentials

Now we consider a cluster of general MT-potentials V^i, each characterized by a K-matrix K^i yielding scattering states ϕ^i_λ. The envelopping spheres may overlap or not, but the potentials itself of course don't overlap. This latter non-overlapping condition is important and will be used actively. Inserting the total potential $V = \sum_i V^i$ into (2.9) or

$$K = V + VG^\circ V + VG^\circ VG^\circ V + \ldots \tag{3.1}$$

yields (see for example [10,13])

$$K = \sum_i K^i + \sum_{i,i'} K^i (1-\delta_{ii'}) G^\circ K^{i'} + \sum_{i,i',i''} K^i (1-\delta_{ii'}) G^\circ K^{i'} (1-\delta_{i'i''}) G^\circ K^{i''} + \ldots \tag{3.2}$$

Because the potentials V^i don't overlap, also the K^i-matrices don't overlap. Therefore and owing to the factors $(1-\delta_{ii'})$ both integrations belonging to each Green's function are running over different volumes. This allows to replace G° the following expansion

$$(1-\delta_{ii'})G^\circ(\vec r - \vec r') \to \sum_{\lambda,\lambda'} j^i_\lambda(\vec r)\kappa N^{ii'}_{\lambda\lambda'} j^{i'}_{\lambda'}(\vec r')$$

for $\vec r \in V_i$ and $\vec r' \in V_{i'}$, (3.3)

as proved in Appendix 1. The structure matrix $N^{ii'}_{\lambda\lambda'}$, involved in (3.3), follows from the wave functions ϕ^i_λ and $\phi^{i'}_{\lambda'}$ and its normal derivatives along the surfaces of V_i and $V_{i'}$, respectively, via corresponding surface integrations (see [4] eq. (A2.3)):

$$N^{ii'}_{\lambda\lambda'} = (1-\delta_{ii'}) \frac{\kappa}{\sin\eta^i_\lambda} \oint_{(V_i)} df \left[\frac{\partial\phi^i_\lambda(\vec r)}{\partial\vec r} - \phi^i_\lambda(\vec r)\frac{\partial}{\partial\vec r}\right] \frac{\kappa}{\sin\eta^{i'}_{\lambda'}} \oint_{(V_{i'})} df' \left[\frac{\partial\phi^{i'}_{\lambda'}(\vec r')}{\partial\vec r'} - \phi^{i'}_{\lambda'}(\vec r')\frac{\partial}{\partial\vec r'}\right] \frac{1}{4\pi} n_0(\kappa|\vec r - \vec r'|). \tag{3.4}$$

(3.3) generalizes the known expansion of G°, valid in the case of non-overlapping envelopping spheres. In this latter case (3.4) can be reduced via

$$N^{ii'}_{\lambda\lambda'} = \sum_{L,L'} \tilde{\tilde{A}}^i_{\lambda L} N^{ii'}_{LL'} A^{i'}_{L'\lambda'},$$

$$N^{ii'}_{LL'} = (1-\delta_{ii'})4\pi \sum_{L''} C_{LL'L''}\, i^{\ell-\ell'+\ell''} n_{L''}(\vec R_{ii'}) \tag{3.5}$$

to the structure matrix $N^{ii'}_{LL'}$, which is much more simple than (3.4), because it involves only the centres of the spheres, R_i. In the general case of overlapping envelopping spheres this reduction (3.5) is not possible and the more or less complicated near field properties of the single MT-potentials V^i appear, described by ϕ^i_λ and $\partial\phi^i_\lambda/\partial n$ along the surface of V_i. With

$$(j^i_\lambda, K^i j^i_{\lambda'}) = \sum_{L,L'} A^i_{\lambda L} K^i_{LL'} A^i_{L'\lambda'} = K^i_\lambda \delta_{\lambda\lambda'} \tag{3.6}$$

and

$$j_L(\vec{r}) = \sum_{\lambda} j^i_{\lambda}(\vec{r}) J^{i0}_{\lambda L} \qquad (3.7)$$

immediately follows from (3.2) and (3.3) the K-matrix of the cluster

$$K_{LL'} = \sum_{\substack{i,\lambda \\ i',\lambda'}} J^{0i}_{L\lambda} (M^{-1})^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} J^{i'0}_{\lambda' L'}, \qquad (3.8)$$

$$M^{ii'}_{\lambda\lambda'} \equiv \delta_{ii'} \delta_{\lambda\lambda'} - \kappa K^i_{\lambda} N^{ii'}_{\lambda\lambda'},$$

As (3.8) shows the structure matrix $N^{ii'}_{\lambda\lambda'}$ is responsible for the multiple scattering between the MT-potentials. Its neglect means, that the $\underline{K}$-matrices of the MT-potentials (related to the origin) are simple superposed additively. If (3.5) can be applied, then (3.8) takes the form

$$K_{LL'} = \sum_{\substack{i,L_1 \\ i',L_2,L_3}} J^{0i}_{LL_1} (M^{-1})^{ii'}_{L_1L_2} K^{i'}_{L_2L_3} J^{i'0}_{L_3L'}, \qquad (3.9)$$

$$M^{ii'}_{LL'} \equiv \delta_{ii'} \delta_{LL'} - \kappa \sum_{L_1} K^i_{LL_1} N^{ii'}_{L_1L'}.$$

This agress completely with the results of Lloyd (1969, 1972) only with the difference, that the single scatterer K-matrices on the energy shell, $K^i_{LL'}$, here are expressed explicitly by their eigenvalues K^i_{λ} and their eigenvectors $A^i_{L\lambda}$, that is $K^i_{LL'} = \sum A^i_{L\lambda} K^i_{\lambda} A^i_{\lambda L'}$, corresponding to (2.13). In the special case of spherically symmetric scatterers their K-matrices are diagonal, $K^i_{LL'} = \delta_{LL'} K^i_L$, and (3.9) simplifies to (2.25), in agreement with /5/ and /11/.

The eigenstates of the cluster K-matrix,

$$\sum_{L'} K_{LL'} B_{L'\mu} = B_{L\mu} K_{\mu}, \qquad (3.10)$$

determine the asymptotic or far field parameters of the cluster. Because $K_{LL'}$ is a real and symmetric matrix, the amplitudes $B_{L\mu}$ form an orthogonal and complete set

$$\sum_L \tilde{\tilde{B}}_{\mu L} B_{L\mu'} = \delta_{\mu\mu'}, \quad \sum_{\mu} B_{L\mu} \tilde{\tilde{B}}_{\mu L'} = \delta_{LL'}. \qquad (3.11)$$

Therefore also

$$K_{\mu} = \sum_{L,L'} \tilde{\tilde{B}}_{\mu L} K_{LL'} B_{L'\mu}, \quad K_{LL'} = \sum_{\mu} B_{L\mu} K_{\mu} \tilde{\tilde{B}}_{\mu L'} \qquad (3.12)$$

holds.

The trivial scattering states (with $K_{\mu} = 0$) are also included in (3.10). Form (3.8) and (3.10) follows, that they obtain the condition

$$\sum J^{i0}_{\lambda L} B_{L\mu} = 0 \text{ for } K^i_{\lambda} \neq 0. \qquad (3.13)$$

This allows, to represent the projection operator of the non-trivial scattering states in the following form

$$\sum_{\substack{\mu \\ (K_{\mu} \neq 0)}} B_{L\mu} B_{\mu L'} = \sum_{\substack{i,\lambda (K_{\lambda} \neq 0) \\ i',\lambda' (K^{i'}_{\lambda'} \neq 0)}} J^{0i}_{L\lambda} (J^{-1})^{ii'}_{\lambda\lambda'} J^{i'0}_{\lambda' L'}. \qquad (3.14)$$

This is proved in Appendix 2.

From (3.8) and (3.10) it also follows, that the non-trivial scattering states (with $K_{\mu} \neq 0$) obtain just the cluster equations, derived in /4/ by an KKR-like approach:

$$\sum_{i',\lambda'} \left[M^{ii'}_{\lambda\lambda'} - K^i_{\lambda} K^{-1}_{\mu} J^{ii'}_{\lambda\lambda'} \right] B^{i'}_{\lambda'\mu} = 0. \qquad (3.15)$$

Here the abbreaviation

$$B^i_{\lambda\mu} \equiv \begin{cases} \sum\limits_{i',\lambda' (K^i_{\lambda} \neq 0)} (J^{-1})^{ii'}_{\lambda\lambda'} J^{i'0}_{\lambda' L} B_{L\mu} & \text{for } K^i_{\lambda} \neq 0 \\ 0 & \text{for } K^i_{\lambda} = 0 \end{cases} \qquad (3.16)$$

is used. This shows together with (3.14), that vice versa the far field amplitudes $B_{L\mu}$ can be calculated from the near field amplitudes $B^i_{\lambda\mu}$ via

$$B_{L\mu} = \sum_{i,\lambda} J^{0i}_{L\lambda} B^i_{\lambda\mu} . \qquad (3.17)$$

This again shows together with (3.11) and (3.14) , that the near field amplitudes $B^i_{\lambda\mu}$ are ''orthogonal'' and ''complete'' in the following sense

$$\sum_{\substack{i,\lambda \\ i',\lambda'}} B^i_{\mu\lambda} J^{ii'}_{\lambda\lambda'} B^{i'}_{\lambda'\mu'} = \delta_{\mu\mu'} , \quad \sum_{\mu} B^i_{\lambda\mu} \tilde{\tilde{B}}^{i'}_{\mu\lambda'} = (J^{-1})^{ii'}_{\lambda\lambda'} . \qquad (3.18)$$

Finally, in this i–λ – representation we have

$$K_\mu = \sum_{\substack{i,\lambda \\ i',\lambda'}} B^i_{\mu\lambda} (M^{-1})^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} B^{i'}_{\lambda'\mu'} ,$$

$$(M^{-1})^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} = \sum_{\lambda} B^i_{\lambda\mu} K_\mu \tilde{\tilde{B}}^{i'}_{\mu\lambda'} \qquad (3.19)$$

instead of (3.12).

According to (2.16) the wave function outside the MT-potentials has next-to the form

$$\phi_\mu = \sum_L j_L B_{L\mu} \cos\eta_\mu + \sum_{\substack{i,\lambda \\ i',\lambda' \\ L}} n^i_\lambda \kappa (M^{-1})^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} J^{i'0}_{\lambda' L} B_{L\mu} \cos\eta_\mu . \qquad (3.20)$$

This is similarly derived as (3.8), using (3.3) and (A1.1). With (3.10), (3.16), (3.7) and (3.17) the wave function takes the form (in agreement with (3.2) of /4/)

$$\phi_\mu = \sum_{i,\lambda} [j^i_\lambda B^i_{\lambda\mu} \cos\eta_\mu - n^i_\lambda B^i_{\lambda\mu} \sin\eta_\mu] . \qquad (3.21)$$

This describes the wave function not only in the far field region outside the envelopping sphere, but also in the near field region inside this sphere.

If the cluster consists of subclusters, then we have instead of (3.8)

$$K_{LL'} = \sum_{\substack{i,n_i,\lambda \\ i',n'_i,\lambda'}} J^{0\,in_i}_{L\lambda} (M^{-1})^{in_i\,i'n'_i}_{\lambda\lambda'} K^{i'n'_i}_{\lambda'} J^{i'n'_i0}_{\lambda' L'} ,$$

$$M^{in_i\,i'n'_i}_{\lambda\lambda'} \equiv \delta_{ii'} \delta_{n_i n'_i} \delta_{\lambda\lambda'} - \kappa K^{in_i}_{\lambda} N^{in_i\,i'n'_i}_{\lambda\lambda'} . \qquad (3.22)$$

with an artificial double enumeration. Here $N^{in_i\,i'n'_i}_{\lambda\lambda'}$ is responsible for the multiple scattering between the MT-potential n_i of the subcluster i and the MT-potential $n'_{i'}$ of the subcluster i'. Splitting this quantity according to

$$N^{in_i\,i'n'_i}_{\lambda\lambda'} = \delta_{ii'} N^{in_i\,in'_i}_{\lambda\lambda'} + (1 - \delta_{ii'}) N^{in_i\,i'n'_i}_{\lambda\lambda'} \qquad (3.23)$$

into one part, describing the multiple scattering within the subclusters, and another part, describing the multiple scattering between the subclusters, we can rewrite (3.22) as

$$M^{in_i\,i'n'_i}_{\lambda\lambda'} = M^{n_i n'_i}_{\lambda\lambda'} [\delta_{ii'} \delta_{n_i n'_i} \delta_{\lambda\lambda'} - \qquad (3.24)$$

$$- \sum_{n''_i,\lambda''} (M^{-1})^{n_i n''_i}_{\lambda\lambda''} K^{in''_i}_{\lambda''} \kappa (1 - \delta_{ii'}) N^{in''_i\,i'n'_i}_{\lambda''\lambda'}] .$$

Introducing explicitly the subcluster quantities K^i_μ and $B^{in_i}_{\lambda\mu}$ then by means of

$$\sum_\mu B^{in_i}_{\lambda\mu} K^i_\mu B^{in'_i}_{\mu\lambda'} = (M^{-1})^{n_i n'_i}_{\lambda\lambda'} K^{in'_i}_{\lambda'} , \qquad (3.25)$$

which corresponds to (3.19), and

$$N^{ii'}_{\mu\mu'} = (1-\delta_{ii'}) \sum_{\substack{n_i,\lambda \\ n'_i,\lambda'}} \tilde{B}^{in_i}_{\mu\lambda} N^{in_i\, i'n'_i}_{\lambda\,\lambda'} B^{i'n'_i}_{\lambda'\mu'}$$

$$J^{0i}_{L\mu} = \sum_{n_i,\lambda} J^{0in_i}_{L\lambda} B^{in_i}_{\lambda\mu} \tag{3.26}$$

the K-matrix of the whole cluster takes the form

$$K_{LL'} = J^{0i}_{L\mu} (M^{-1})^{ii'}_{\mu\mu'} K^{i'}_{\mu'} J^{i'0}_{\mu'L'},$$

$$M^{ii'}_{\mu\mu'} = \delta_{ii'}\delta_{\mu\mu'} - \kappa K^{i}_{\mu} N^{ii'}_{\mu\mu'} \tag{3.27}$$

in agreement with (3.8). The equivalence of (3.22) and (3.27) shows, that the multiple scattering within a cluster is fully taken into account, if the multiple scattering within arbitrary subclusters and between these subclusters, forming the whole cluster, is also fully taken into account.

All the considerations above can be performed also within the language of the T-matrix. So the T-matrix of a cluster can be obtained in analogy with (3.1...8) directly from (2.8). Inserting (3.8) into (2.12) and using (A2.1) yields of course the same result

$$T_{LL'} = \sum_{\substack{i,\lambda \\ i',\lambda'}} J^{0i}_{L\lambda} (R^{-1})^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} J^{i'0}_{\lambda'L'},$$

$$R^{ii'}_{\lambda\lambda'} \equiv \delta_{ii'}\delta_{\lambda\lambda'} - \kappa K^{i}_{\lambda} (N^{ii'}_{\lambda\lambda'} - i J^{ii'}_{\lambda\lambda'}), \tag{3.28}$$

which by the way can be rewritten with $K^i_\lambda = T^i_\lambda (1 - i\kappa T^i_\lambda)^{-1}$ also as

$$T_{LL'} = \sum_{\substack{i,\lambda \\ i',\lambda'}} J^{0i}_{L\lambda} (Q^{-1})^{ii'}_{\lambda\lambda'} T^{i'}_{\lambda'} J^{i'0}_{\lambda'L'},$$

$$Q^{ii'}_{\lambda\lambda'} \equiv \delta_{ii'}\delta_{\lambda\lambda'} - \kappa T^{i}_{\lambda} (N^{ii'}_{\lambda\lambda'} - i J^{ii'}_{\lambda\lambda'} + i\delta_{ii'}\delta_{\lambda\lambda'}). \tag{3.29}$$

Because K and T have the same eigenvectors $B_{L\mu}$, the cluster equations following from (3.28) or (3.29) are of course equivalent with (3.15).

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Appendix 1. Proof of the Replacement (3.3)

In /4/ (see eqs. (2.11) and (3.3)) it has been shown

$$n^i_\lambda K^i_\lambda = \frac{1}{4\pi} n_0 K^i j^i_\lambda, \tag{A1.1}$$

$$(1-\delta_{ii'}) n^{i'}_{\lambda'}(\vec{r}) = \sum_\lambda j^i_\lambda(\vec{r}) N^{ii'}_{\lambda\lambda'} \quad \text{for } \vec{r} \in V_i \tag{A1.2}$$

Therefore immediately

$$(1-\delta_{ii'}) G^\circ K^{i'} j^{i'}_{\lambda'} = (1-\delta_{ii'}) \kappa n^{i'}_{\lambda'} K^{i'}_{\lambda'} =$$

$$= \kappa \sum_\lambda j^i_\lambda N^{ii'}_{\lambda\lambda'} K^{i'}_{\lambda'} j^{i'}_{\lambda'} \tag{A1.3}$$

follows. With $K^{i'}_{\lambda'} = (j^{i'}_{\lambda'}, K^{i'} j^{i'}_{\lambda'})$ the replacement (3.3) is proved, q.e.d.

Appendix 2. The Projection Operator of the Non-Trivial Scattering States

(3.14) is proved in the following way: Abbreviating the right hand side of (3.14) with $P_{LL'}$ and acting on a trivial scattering state $B_{L\mu}$ (with $K_\mu = 0$), yields really $\Sigma P_{LL'} B_{L'\mu} = 0$ owing to (3.13). The non-trivial scattering states $B_{L\mu}$ (with $K_\mu \neq 0$) obtain the relation

$$\sum_{L'} P_{LL'} B_{L'\mu} = \sum_{L'} P_{LL'} B_{L'\mu} \frac{K_\mu}{K_\mu} = \sum_{L',L''} P_{LL'} K_{L'L''} B_{L''\mu} \frac{1}{K_\mu} \qquad \text{(A2.1)}$$

$$= \sum_{L''} K_{LL''} B_{L''\mu} \frac{1}{K_\mu} = B_{L\mu}$$

Here $PK = K$ has been used, following directly from the definitions of K and P and from

$$\sum_{L} J^{i0}_{\lambda L} J^{0i'}_{L\lambda'} = J^{ii'}_{\lambda\lambda'} . \qquad \text{(A2.2)}$$

(A2.2) is a consequence of the definition of J (see [4], eq. (3.6)).

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