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Note

On the Calculation of Combined Corrections in the LMTO Method

1. INTRODUCTION

The LMTO method proposed by O. K. Andersen [1] is the most efficient tool for computing the electron properties of solids in the formalism of density functional. In the simplest version of the method a real unit cell is substituted with an atomic sphere of the same volume (atomic sphere approximation, ASA) with spheric potential and electron density. The ASA can be improved if we take into account the real form of a cell, i.e., compute the combined corrections (CC) to the ASA. The improvement is important for calculations of optical properties [2], for disordered systems, etc.

The usual way to compute these corrections is to do some summation in the reciprocal space [1] and to store the correspondent coefficients in computer memory. But it have been found that the CC can be computed in the direct space via the standard structure constants of the LMTO method [3]. Following Andersen [4] we have derived the expressions for the CC which are always suitable for the systems with broken translational symmetry. Our notations are almost equivalent to [1, 4].

2. REAL SPACE REPRESENTATION FOR THE COMBINED CORRECTIONS

Let us discuss the muffin-tin tesselation of some solid (Fig. 1). We can surround each atom with an arbitrary cell envelope by Wigner–Seitz procedure. In general, it would be the Voronoi polyhedra (for disordered systems). The MT-orbitals $\chi_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$ are attributed to every atom with the origin at $\mathbf{R}$, where $\mathbf{r}_{\mathbf{R}}=\mathbf{r}-\mathbf{R}$ and $L=lm$ is an orbital quantum number and its projection. In ASA we neglect the contribution from the interstitial region. Then the combined correction to the Hamiltonian $H_{\mathbf{R}'L'\mathbf{R}L}$ and overlap matricies $O_{\mathbf{R}L'\mathbf{R}L}$, calculated in ASA takes the form

$$\Delta O_{\mathbf{R}'L'\mathbf{R}L}=[\chi_{\mathbf{R}'L'}|\chi_{\mathbf{R}L}]=\{\chi_{\mathbf{R}'L'}|\chi_{\mathbf{R}L}\}-\langle\chi_{\mathbf{R}'L'}|\chi_{\mathbf{R}L}\rangle,$$

$$\Delta H_{\mathbf{R}'L'\mathbf{R}L}=\mathbf{v}_{\mathbf{R}'\mathbf{R}}[\chi_{\mathbf{R}'L'}|\chi_{\mathbf{R}L}].$$

Here $\{\cdots\}$ and $\langle\cdots\rangle$ mean the integral over the whole space and atomic spheres, respectively, $\mathbf{v}_{\mathbf{R}'\mathbf{R}}$ is the average value of the potential in the interstitial

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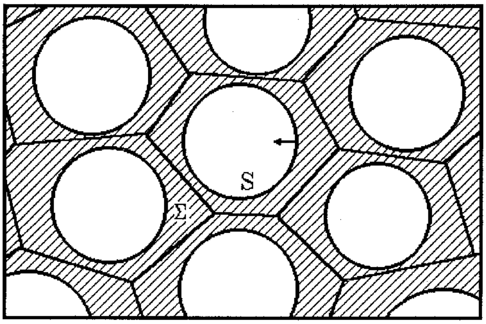

FIG. 1. The Voronoi tesselation of the crystal potential. The dashed area is an interstitial space with constant potential. S is a surface of spheridized MT-potential, and Σ is a boundary of Voronoi polyhedra.

region. O. K. Andersen has proposed to use the zero value of electron kinetic energy in the interstitial region, $\kappa^2=0$, afterwards in this region MTO equals $\chi_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=\chi_{Rl}(D_L)(s_R/r_R)^{l+1}\, i^l Y_L(\mathbf{r}_R)$, where $\chi_{Rl}(D_L)$ is the value of MTO on the atomic sphere of radius $s_{\mathbf{R}}$ and $Y_L(\mathbf{r}_{\mathbf{R}})$ is the usual spherical harmonic, $r_R=|\mathbf{r}-\mathbf{R}|$ [1]. We introduce the set of orbitals $N_{\mathbf{R}L}(\mathbf{r}_R)$ from expression $\chi_{\mathbf{R}L}(\mathbf{r}_R)=\chi_{\mathbf{R}l}(D_L)(s_{\mathbf{R}}/w)^{1/2}\, N_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$, where w is the mean radius of the atomic sphere. Then we get

$$[\chi_{\mathbf{R}'L'}\,|\,\chi_{\mathbf{R}L}]=\chi_{\mathbf{R}'l'}(D_{L'})(s_{\mathbf{R}'}/w)^{1/2}\,[N_{\mathbf{R}'L'}\,|\,N_{\mathbf{R}L}](s_{\mathbf{R}}/w)^{1/2}\,\chi_{\mathbf{R}l}(D_L). \tag{1}$$

We have used the standard expansion for $N_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$,

$$N_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=N_{\mathbf{R}'L'}(\mathbf{r}_{\mathbf{R}'})\,\delta_{\mathbf{R}'L'\mathbf{R}L}-\sum_{L'} J_{\mathbf{R}'L'}(\mathbf{r}_{R'})\,S_{\mathbf{R}'L'\mathbf{R}L},$$

where $J_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=[2(2l+1)]^{-l}\,(r_{\mathbf{R}}/w)^l\, i^l Y_L(\mathbf{r}_{\mathbf{R}})$. The set of coefficients $S_{\mathbf{R}'L'\mathbf{R}L}$ are the standard structure constants of the LMTO method [1]:

$$\begin{aligned}S_{\mathbf{R}'L'\mathbf{R}L}= & -2(4\pi)^{1/2}\,(s_{\mathbf{R}'}/w)^{l'+1/2}\,(s_{\mathbf{R}}/w)^{l+1/2}\,\frac{(2l''-1)!!}{(2l-1)!!\,(2l'-1)!!}\\ & \cdot C_{LL'L''}(w/|\mathbf{R}-\mathbf{R}'|)^{l''+1}\,[(4\pi)^{1/2} i^{l''} Y_{L''}(\mathbf{R}-\mathbf{R}')]^*,\end{aligned} \tag{2}$$

where $C_{LL'L''}=\int d\mathbf{n}\, Y_L(\mathbf{n})\, Y^*_{L'}(\mathbf{n})\, Y_{L''}(\mathbf{n})$ are the Gaunt coefficients. The orbitals $N_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$ and $J_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$ we can treat as a special case of more general set $\mathcal{N}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$ and $\mathcal{J}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$ which are the eigenfunctions of Helmholz operator $(\nabla^2+\kappa^2)$. In explicit form

$$\mathcal{N}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=-(w/s_{\mathbf{R}})^{1/2}\,(\kappa s_{\mathbf{R}})^{l+1}\, n_l(\kappa\mathbf{r}_{\mathbf{R}})\, Y_L(\mathbf{r}_{\mathbf{R}})/(2l-1)!!, \tag{3a}$$

$$\mathcal{J}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=(w/s_{\mathbf{R}})^{1/2}\,(2l-1)!!\, j_l(\kappa\mathbf{r}_{\mathbf{R}})\, Y_L(\mathbf{r}_{\mathbf{R}})/2\,(\kappa s_{\mathbf{R}})^l, \tag{3b}$$

where the n_l and j_l are the spherical Bessel functions. For MTO $\mathcal{N}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})$, we have the expansion formula

$$\mathcal{N}_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}})=\mathcal{N}_{\mathbf{R}'L'}(\mathbf{r}_{\mathbf{R}'})\,\delta_{\mathbf{R}'L'\mathbf{R}L}-\sum_{L'}\mathcal{J}_{\mathbf{R}'L'}(\mathbf{r}_{\mathbf{R}'})\,\mathcal{S}_{\mathbf{R}'L'\mathbf{R}L}, \tag{4}$$

Now we can use the Green identity for new set and afterwards go to the limit $\kappa^2\to 0$. We implement the Green identity to the interstitial region (which is dashed on the figure) for the MTOs $\mathcal{N}_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}})$ and $\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})$,

$$\int_I dv[\mathcal{N}^*_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}'})\,\nabla^2\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})-\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})\,\nabla^2\,\mathcal{N}^*_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}'})]$$
$$=\int_{S+\Sigma}d\mathbf{s}[\mathcal{N}^*_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}'})\,\nabla\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})-\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})\,\nabla\mathcal{N}^*_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}'})].$$

There s and Σ means the integration over an AS surface and the cell boundary, subsequently. Integrals over Σ compensate for each other and for integrals over an AS surface we use Eq. (4). Using the property $\nabla^2\mathcal{N}_{\mathbf{R}L}=-\kappa^2\mathcal{N}_{\mathbf{R}L}$, we get the equality

$$(\kappa_1^2-\kappa^2)\int_I dv\,\mathcal{N}^*_{\mathbf{R}'L'}(\kappa_1^2,\mathbf{r}_{\mathbf{R}'})\,\mathcal{N}_{\mathbf{R}L}(\kappa^2,\mathbf{r}_{\mathbf{R}})=-\sum_{\mathbf{R}''}W\{\mathcal{N}_{\mathbf{R}'L'},\mathcal{N}_{\mathbf{R}L}\}, \tag{5}$$

where the Wronskian W is determined as $W\{f,g\}=s^2f(s)\,g(s)[D(s)-D(f)]$, $D(s)=s(df/dr)/f(s)$, $r=s$. Afterwards we take the limit $\kappa_1^2\to 0$ in Eq. (5), differentiate it over $\kappa^2\to 0$, and use Eq. (4). Hence we get the main result

$$[N_{\mathbf{R}'L'}|N_{\mathbf{R}L}]=-W\{\dot{N},N\}_{\mathbf{R}}\,\delta_{\mathbf{R}'L'\mathbf{R}L}+S_{\mathbf{R}'L'\mathbf{R}L}\,W\{\dot{N},J\}_{\mathbf{R}}+W\{\dot{J},N\}_{\mathbf{R}'}\,S_{\mathbf{R}'L'\mathbf{R}L}$$
$$+W\{J,N\}_{\mathbf{R}}\,\dot{S}_{\mathbf{R}'L'\mathbf{R}L}-\sum_{\mathbf{R}''L''}S_{\mathbf{R}'L'\mathbf{R}''L''}W\{\dot{J},J\}_{\mathbf{R}''}\,S_{\mathbf{R}''L''\mathbf{R}L}.$$

Here a subscript near the Wronskian indicates the site where it is calculated. Using Eq. (3) we get the important relation

$$w^3[N_{\mathbf{R}'L'}|N_{\mathbf{R}L}]=\frac{1}{2l-1}\,(s_{\mathbf{R}}/w)^2\,\delta_{\mathbf{R}'L'\mathbf{R}L}+\left[\frac{1}{4(2l+1)}\,(s_{\mathbf{R}}/w)^2+\frac{1}{4(2l'+1)}\,(s_{\mathbf{R}'}/w)^2\right]$$
$$\times S_{\mathbf{R}'L'\mathbf{R}L}-\frac{1}{2}\,w^{-2}\dot{S}_{\mathbf{R}'L'\mathbf{R}L}$$
$$-\sum_{\mathbf{R}''L''}S_{\mathbf{R}'L'\mathbf{R}''L''}(s_{\mathbf{R}''}/w)^2\,\frac{1}{4(2l''+1)^2\,(2l''+3)}\,S_{\mathbf{R}''L''\mathbf{R}L}. \tag{6}$$

This equation together with Eq. (1) gives the value of LMTO combined corrections via $S_{\mathbf{R}'L'\mathbf{R}L}$ and $\dot{S}_{\mathbf{R}'L'\mathbf{R}L}=(dS_{\mathbf{R}'L'\mathbf{R}L}/d\kappa^2)_{\kappa^2\to 0}$.

In the case of a crystal lattice the combined corrections of a type $[N^{\mathbf{k}}_{\mathbf{q}'L'} | N^{\mathbf{k}}_{\mathbf{q}L}]$ are needed, where $N^{\mathbf{k}}_{\mathbf{q}L} = \Sigma_{\mathbf{R}} N_{\mathbf{R}L}(\mathbf{r}_{\mathbf{R}}) \exp(i\mathbf{kR})$ are the Bloch sums and $\mathbf{q}$ is the position of atom in a basis. After Bloch summing in Eq. (6) we immediately get the final expression for CC,

$$
\begin{aligned}
w^{-3}[N^{\mathbf{k}}_{\mathbf{q}'L'} | N^{\mathbf{k}}_{\mathbf{q}L}] = {} & \frac{1}{2l-1} (s_{\mathbf{q}}/w)^2 \, \delta_{\mathbf{q}'L'\mathbf{q}L} + \left[\frac{1}{4(2l+1)} (s_{\mathbf{q}}/w)^2 + \frac{1}{4(2l'+1)} (s_{\mathbf{q}'}/w)^2 \right] \\
& \times S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} - \frac{1}{2} w^{-2} \dot{S}^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} \\
& - \sum_{\mathbf{q}''L''} S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}''L''} (s_{\mathbf{q}''}/w)^2 \frac{1}{4(2l''+1)^2 \, (2l''+3)} S^{\mathbf{k}}_{\mathbf{q}''L''\mathbf{q}L},
\end{aligned}
\tag{7}
$$

where $S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L}$ are the structure constants defined by Eq. (1), $S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} = \sum_{\mathbf{T}} S_{\mathbf{R}'L'\mathbf{R}L} \exp(i\mathbf{kT})$, $\mathbf{T}$ is a vector of translation.

Introducing vectors $\mathbf{\Delta} = \mathbf{R} - \mathbf{R}' = \mathbf{T} - \boldsymbol{\delta}$, $\boldsymbol{\delta} = \mathbf{q}' - \mathbf{q}$ we can write

$$
\begin{aligned}
\mathscr{S}_{\mathbf{R}'L\mathbf{R}L}(\kappa^2) = {} & \frac{8\pi}{(2l-1)!! \, (2l'-1)!!} (s_{\mathbf{R}'}/w)^{l'+1/2} (s_{\mathbf{R}}/w)^{l+1/2} \\
& \times \sum_{L''} C_{LL'L''} (\kappa w)^{l+l'+1} n_{l''}(\kappa \Delta) \, i^{-l''} Y^{*}_{L''}(\mathbf{\Delta}),
\end{aligned}
\tag{8}
$$

where $L'' = l''m''$, $l'' = |l-l'|$, $|l-l'|+2, ..., l+l'$, and $m'' = m' - m$. After differentiation of Eq. (8) and taking limit $\kappa^2 \to 0$ the only remaining terms in the sum will be $l'' = l + l'$ and $l'' = l + l' - 2$,

$$
w^{-2} \dot{S}_{\mathbf{R}'L'\mathbf{R}L} = (s_{\mathbf{q}'}/w)^{l'+1/2} (s_{\mathbf{q}}/w)^{l+1/2} g_{L'L} f_{LL'L''}(\Delta) [(4\pi)^{1/2} i^{l''} Y_{L''}(\mathbf{\Delta})]^{*}, \tag{9a}
$$

where

$$
\begin{aligned}
f_{LL'L''} = {} & -(\Delta/2w) \, \delta_{l0} \delta_{l'0} \delta_{l''0} + \frac{1}{2(2l''-1)} (w/\Delta)^{l''-1} \delta_{l'',l+l'} (1 - \delta_{l''0}) \\
& \times (w/\Delta)^{l''-1} \, \delta_{l'',l+l'-2} \theta(l'' - |l-l'|),
\end{aligned}
\tag{9b}
$$

where $\theta(x) = 1$ when $x \geqslant 0$ and $\theta(x) = 0$ when $x < 0$. It should be noted that S has the term $l = l' = l'' = 0$ which increases with the distance as $|\mathbf{R} - \mathbf{R}'|/w$. It can be circumvented in the case of a crystal if we use the Ewals summation technique [6]. Namely, let us write the relation between the LMTO structure constants $S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L}$ [1] and KKR ones $A^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L}$ [6, 7],

$$
S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} = \lim_{\kappa^2 \to 0} \frac{2}{\kappa} \frac{1}{(2l-1)!! \, (2l'-1)!!} (\kappa s_{\mathbf{q}'})^{l'+1/2} (\kappa s_{\mathbf{q}})^{l+1/2} A^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L}(\kappa^2), \tag{10a}
$$

where

$$
A^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} = 4\pi \sum_{L''} i^{-1''} C_{LL'L''} D^{\mathbf{k}}_{LL'L''}(\kappa^2). \tag{10b}
$$

The KKR constants $D^{\mathbf{k}}_{LL'L''}$ are simply evaluated with the Ewald technique [6]. After differentiation in (10) and taking the limit $\kappa^2 \to 0$ we get the result,

$$w^{-2}\dot{S}^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} = (s_{\mathbf{q}'}/w)^{l'+1/2}\,(s_{\mathbf{q}}/w)^{l+1/2}\exp[i\mathbf{k}(\mathbf{q}'-\mathbf{q})]$$
$$\times\,[g_{L'L,\,l''=l+l'-2}\textstyle\sum^{\mathbf{k}}_{\mathbf{q}'-\mathbf{q}\,l+l'-2\,m'-m}+g_{L'L,\,l''=l+l'}\bar{\sum}^{\mathbf{k}}_{\mathbf{q}'-\mathbf{q}\,l+l'\,m'-m}], \tag{11a}$$

where $\sum^{\mathbf{k}}_{\mathbf{q}'-\mathbf{q}\,l+l'-2m'-m}$ and $\bar{\sum}^{\mathbf{k}}_{\mathbf{q}'-\mathbf{q}\,l+l'm'-m}$ are the standard LMTO dimensionless structure constants (see Eq. (4.48) in [1]) and the modified one, respectively.

The Ewald form [6] that we have used for standard structure constants $\sum^{\mathbf{k}}_{\boldsymbol{\delta}\lambda\mu}$ is

$$\sum\nolimits^{\mathbf{k}}_{\boldsymbol{\delta}\lambda\mu} = \frac{8\pi^{3/2}\,w^3}{(2\lambda-1)!!\,\Omega_c}\sum_{\mathbf{g}}\exp(i\mathbf{g}\boldsymbol{\delta})(w\,|\mathbf{k}+\mathbf{g}|)^{\lambda-2}\,\sigma_{\mathbf{k}+\mathbf{g}}\,Y^*_{\lambda\mu}(\mathbf{k}+\mathbf{g})$$
$$+\frac{4(-2i)^\lambda}{(2\lambda-1)!!}\sum_{\mathbf{T}}\exp(i\mathbf{k}\boldsymbol{\Delta})(w/\Delta)^{\lambda+1}\,Y^*_{\lambda\mu}(\boldsymbol{\Delta})\int_{\eta\Delta}^{\infty}d\xi\,\xi^{2\lambda}\exp(-\xi^2)$$
$$-2\eta w\delta_{\lambda 0}\delta_{\mathbf{q}'\mathbf{q}}/\pi^{1/2}, \tag{11b}$$

and, for modified structure constants $\bar{\sum}^{\mathbf{k}}$, we get the similar expression ($\lambda \geqslant |l-l'|$):

$$\bar{\sum}\nolimits^{\mathbf{k}}_{\boldsymbol{\delta}\lambda\mu} = \frac{8\pi^{3/2}w^3}{(2\lambda-1)!!\,\Omega_c}\sum_{\mathbf{g}}\exp(i\mathbf{g}\boldsymbol{\delta})(w\,|\mathbf{k}+\mathbf{g}|)^{\lambda-4}$$
$$\cdot\,[1+|\mathbf{k}+\mathbf{g}|^2/4\eta^2]\,\sigma_{\mathbf{k}+\mathbf{g}}\,Y^*_{\lambda\mu}(\mathbf{k}+\mathbf{g})$$
$$+\frac{(-2i)^\lambda}{(2\lambda-1)!!}\sum_{\mathbf{T}}\exp(i\mathbf{k}\boldsymbol{\Delta})(w/\Delta)^{l-1}\,Y^*_{\lambda\mu}(\boldsymbol{\Delta})\int_{\eta\Delta}^{\infty}d\xi\,\xi^{2\lambda-2}\exp(-\xi^2)$$
$$+\delta_{\lambda 0}\delta_{\mathbf{q}'\mathbf{q}}/(2\pi^{1/2}\eta w). \tag{11c}$$

Here Ω_c is the volume of unit cell, $\sigma_{\mathbf{k}+\mathbf{g}} = \exp[-(\mathbf{k}+\mathbf{g})^2/4\eta^2]$, η is an Ewald factor, in all sums the term $\boldsymbol{\Delta}=0$ is excluded. For the sake of clarity we can remaind the relation between standard structure contants $S^{\mathbf{k}}$ and $\sum^{\mathbf{k}}$ [1]:

$$w^{-2}S^{\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} = (s_{\mathbf{q}'}/w)^{l'+1/2}\,(s_{\mathbf{q}}/w)^{l+1/2}\exp[i\mathbf{k}(\mathbf{q}'-\mathbf{q})]$$
$$\times\,g_{L'L,\,l''=l+l'}\textstyle\sum^{\mathbf{k}}_{\mathbf{q}'-\mathbf{q}\,l+l'\,m'-m}. \tag{11d}$$

Formulae (1), (7), and (11) allows us to compute the combined corrections concurrently with ASA terms and economize computer storage and speed up calculations. This procedure, where applied in our Fortran code and the computation of CC in the present scheme, has become approximately half as much time and disk storage consuming in comparison with the standard scheme [1].

Almost analogously we can write the combined corrections with the localized MTO s $N^{\alpha\mathbf{k}}_{\mathbf{q}L}$ [5, 5]. So, for the case of a crystal we have

$$
\begin{aligned}
&w^{-3}[N^{\alpha\mathbf{k}}_{\mathbf{q}'L'} \,|\, N^{\alpha\mathbf{k}}_{\mathbf{q}L}] \\
&\quad = \frac{1}{2l-1}(s_{\mathbf{q}}/w)^2\,\delta_{\mathbf{q}'L'\mathbf{q}L} + \left\{\left[\frac{1}{4(2l+1)} + \frac{\alpha_l}{2l-1}\right](s_{\mathbf{q}}/w)^2\right. \\
&\qquad \left. + \left[\frac{1}{4(2l'+1)} + \frac{\alpha_{l'}}{2l'-1}\right](s_{\mathbf{q}'}/w)^2\right\} S^{\alpha\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} - \frac{1}{2}w^{-2}\dot{S}^{\alpha\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}L} \\
&\qquad - \sum_{\mathbf{q}''L''} S^{\alpha\mathbf{k}}_{\mathbf{q}'L'\mathbf{q}''L''}\left\{\left[\frac{1}{4(2l''+1)^2\,(2l''+3)} - \frac{\alpha_{l''}}{2(2l''+1)} - \frac{\alpha^2_{l''}}{2l''-1}\right](s_{\mathbf{q}''}/w)^2\right. \\
&\qquad \left. - \frac{1}{2}w^{-2}\dot{\alpha}_{l''}\right\} S^{\alpha\mathbf{k}}_{\mathbf{q}''L''\mathbf{q}L},
\end{aligned}
$$

where $S^{\alpha\mathbf{k}}$ are the screened structure constants, $\alpha = \alpha_l$ are the screening constants, and $\dot{\alpha}_l$ may be used as free parameters. The term increasing with the distance in Eq. (9) now does not allow one to get the expression for the dotted S-matrix conveniently for computation, so in [4] the authors have used numerical differentiation.

To complete the discussion it is necessary to present the explicit expressions for the coefficients $g_{L'L}$:

$$
g_{L'L} = -2(4\pi)^{1/2}\frac{(2l''-1)!!}{(2l-1)!!\,(2l'-1)!!}\,C_{LL'L''}.
$$

In the case of $l'' = l + l'$, $m'' = m' - m$ they are given in [1]:

$$
\begin{aligned}
&g_{L'L,\,l''=l+l'} = t_{lml'm'l''m''}, \\
&\quad t_{lml'm'l''m''} = (-1)^{m+1}\,2[(2l+1)(2l'+1)(l''+m'')!\,(l''-m'')!]^{1/2} \\
&\qquad\qquad \times [(2l''+1)(l+m)!\,(l-m)!\,(l'+m')!\,(l'-m')!]^{-1/2}.
\end{aligned}
$$

For the case $l'' = l + l' - 2$, $m'' = m' - m$ we obtain

$$
\begin{aligned}
g_{L'L,\,l''=l+l'-2} &= -U_{lml'm'l''m''}\,t_{lml'm'l''m''} \\
&\quad \times [2(2l-1)(2l'-1)(2l''+3)]^{-1},
\end{aligned}
$$

where

$$
\begin{aligned}
U_{lml'm'l''m''} &= (l-m-1)(l-m)(l'-m'-1)(l'-m')\,\theta(l-2-m)\,\theta(l'-2-m') \\
&\quad - 2(l+m)(l-m)(l'+m')(l'-m')\;\theta(l-1-|m|)\,\theta(l'-1-|m'|) \\
&\quad + (l+m-1)(l+m)(l'+m'-1)(l'+m')\,\theta(l-2+m)\,\theta(l'-2+m').
\end{aligned}
$$

3. CONCLUSION

In the present paper we have derived the explicit formulae for the so-called combined corrections to the atomic sphere approximation (ASA) in the LMTO method via structure constants and their energy derivatives suitable for crystals and disordered solids. The Ewald procedure is used to calculate CC for the crystal with an arbitrary basis. The procedure sufficiently economizes the computer time and storage needed. This procedure may be evidently generalized for computing some class of matrix elements with the standard MTO s or the localized ones.

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A. M. BRATKOVSKY

I. V. Kurchatov Institute for Atomic Energy
123182, Moscow, USSR

S. YU. SAVRASOV

P. N. Lebedev Physical Institute
117924, Moscow, USSR