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Screening transformations for two-dimensional structure constants

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ABSTRACT
By making explicit use of the so-called 'Kambe structure constants', originally formulated for a theoretical description of low energy electron diffraction (LEED), the screened KKR surface Green's function (SKKR-SGF) method for layered systems can conceptually be extended to multilayer systems corresponding to complex two-dimensional lattices and to layer relaxation at interfaces (surfaces). In the present paper the screening properties of the 'Kambe structure constants' are illustrated.

§1. INTRODUCTION

According to the translational invariance condition for layered systems (see e.g. Weinberger (1997)) an arbitrary difference vector of $\mathbf{r}$ and $\mathbf{r}'$ can be written as

$$\mathbf{r} - \mathbf{r}' = \mathbf{r}_i - \mathbf{r}_j + \mathbf{R}_{i,\|} - \mathbf{R}_{j,\|} + \mathbf{c}_{ss'}, \tag{1}$$

$$\mathbf{c}_{ss'} = \mathbf{c}_{s,\|} - \mathbf{c}_{s',\|} + \left(c_{s,\perp} - c_{s',\perp}\right)\mathbf{z} \equiv \mathbf{c}_{ss',\|} + c_{ss',\perp}\mathbf{z}, \tag{2}$$

where the $\mathbf{R}_{i,\|}$ are (primitive) two-dimensional lattice vectors, $\mathbf{c}_{s,\|}$ non-primitive two-dimensional lattice vectors, and the $c_{ss',\perp}$ specify the interplane distance. By using two-dimensional translational symmetry and the following notation,

$$\mathbf{r}_s = \mathbf{r}_i + \mathbf{c}_s\ , \qquad \mathbf{r}'_{s'} = \mathbf{r}'_j + \mathbf{c}_{s'}, \tag{3}$$

the so-called structure constants $A^{ss'}_{LL'}(\mathbf{k}_\|, \epsilon)$ are related to the $\mathbf{k}_\|$-projected unperturbed Green's function ('structural Green's function') as follows

$$G^0(\mathbf{r}_s, \mathbf{r}'_{s'}; \mathbf{k}_\|, \epsilon) = \sum_{L,L'} \langle \hat{\mathbf{r}}_s | L \rangle \Big\{ j_\ell(\epsilon^{1/2} r_s) A^{ss'}_{LL'}(\mathbf{k}_\|, \epsilon) j_{\ell'}(\epsilon^{1/2} r'_{s'})$$
$$+ \delta_{ss'}\delta_{LL'}\epsilon^{1/2}\Big(n_\ell(\epsilon^{1/2} r_s) j_{\ell'}(\epsilon^{1/2} r'_{s'})\Big) \langle L' | \hat{\mathbf{r}}'_{s'} \rangle \Big\}, \tag{4}$$

where the $j_\ell(z)$ and $n_\ell(z)$ are spherical Bessel and Neumann functions, respectively, and $\langle \hat{\mathbf{r}} | L \rangle$ denotes spherical harmonics. These structure constants can be evaluated very accurately for layered systems using the approach suggested by Kambe (1967a, b, 1968).

It is important to note that for the 'Kambe structure constants' a parent three-dimensional lattice (see Weinberger (1997)) does not necassarily have to be assumed, i.e. the distances between layers can vary in an appropriate manner such as for example in a multilayer system showing surface (interface) relaxation. These structure constants can be viewed as supermatrices with rows and columns labelled by atomic layers. In the case of a complex two-dimensional lattice each such element is itself a (super-) matrix labelled by sublattices. Applications to a theoretical description of ordering phenomena of interdiffused interfaces are therefore also within reach.

§2. Screening transformations

A screening transformation of the so-called 'real space structure constants' $G^0(\epsilon)$ (see Weinberger (1990)) is defined by the following Dyson equation (Szunyogh *et al.* 1994, Zeller *et al.* 1995)

$$G^{\alpha}(\epsilon) = G^0(\epsilon)\left[1 - \alpha(\epsilon) G^0(\epsilon)\right]^{-1}, \tag{5}$$

where $\alpha(\epsilon)$ is a supermatrix such that

$$\alpha(\epsilon) = \left\{\alpha^{\mathbf{R}}(\epsilon)\delta_{\mathbf{RR}'}\right\}, \quad \alpha^{\mathbf{R}}(\epsilon) = \{\alpha_{\ell}^{R}(\epsilon)\delta_{LL'}\} \tag{6}$$

where $\mathbf{R}$ denotes sites and $L = (\ell m)$. The $\alpha_{\ell}^{R}(\epsilon)$ are usually called screening parameters.

A $\mathbf{k}_{\|}$-like projection of $G^0(\epsilon)$, however, is nothing but the corresponding matrix of the structure constants discussed in the previous section, and referred to as 'Kambe structure constants',

$$P_{\mathbf{k}_{\|}} G^0(\epsilon) = G^0(\mathbf{k}_{\|}, \epsilon) \equiv A(\mathbf{k}_{\|}, \epsilon). \tag{7}$$

In particular from the explicit form of the Dyson equation in (5) it is obvious that a $\mathbf{k}_{\|}$-projection of $G^{\alpha}(\epsilon)$,

$$P_{\mathbf{k}_{\|}} G^{\alpha}(\epsilon) = G^{\alpha}(\mathbf{k}_{\|}, \epsilon), \tag{8}$$

is defined by

$$G^{\alpha}(\mathbf{k}_{\|}, \epsilon) = G^0(\mathbf{k}_{\|}, \epsilon)\left[1 - \alpha(\epsilon) G^0(\mathbf{k}_{\|}, \epsilon)\right]^{-1}, \tag{9}$$

where of course $G^{\alpha}(\mathbf{k}_{\|}, \epsilon)$ is a (super-) matrix of the form

$$G^{\alpha}(\mathbf{k}_{\|}, \epsilon) = \{G^{\alpha}_{ss'}(\mathbf{k}_{\|}, \epsilon)\}; \quad G^{\alpha}_{ss'}(\mathbf{k}_{\|}, \epsilon) = \{G^{\alpha}_{ss',LL'}(\mathbf{k}_{\|}, \epsilon)\}. \tag{10}$$

Equation (9) is then solved such that

$$G^{\alpha}_{ss'}(\mathbf{k}_{\|}, \epsilon) \simeq 0, \qquad c_{ss',\perp} \geq d. \tag{11}$$

Quite clearly the main objective of a screening transformation is to achieve formal tri-diagonality for the structure constants and therefore for the so-called KKR matrix.

§3. Results and discussion

From the previous section one can see that the main task lies in solving the matrix equation in (9). As for an infinite system the matrices involved are also infinite, and one has to use the fact that after screening the scattering length is reduced to a certain number of layers. Taking therefore for every layer under consideration twice this number in order to calculate $G^{\alpha}(\mathbf{k}_{\|},\epsilon)$, occurring cut-off effects can be avoided.

In order to illustrate the effect of screening for the 'Kambe structure constants', it is necessary to define a measure for this effect, e.g. by introducing the following quantity (norm),

$$N_{ss'}(\Delta n) = \sum_{L,L'} \left\{ \left[\mathrm{Re}\, G^{a}_{ss',LL'}(\mathbf{k}_{\|},\epsilon)\right]^2 + \left[\mathrm{Im}\, G^{a}_{ss',LL'}(\mathbf{k}_{\|},\epsilon)\right]^2 \right\}^{1/2}. \quad (12)$$

Since $N_{ss'}$ only depends on the distance Δn between layer s and s', for a parent three-dimensional lattice this distance can be expressed in terms of multiples of the interlayer spacing, i.e. $\Delta n = |s - s'|$.

For the energies -0.1, -0.5 and -1.0 ryd, figures 1–3 show this norm on a logarithmic scale as a function of the layer spacing in a fcc parent lattice. The data shown are normalized with respect to the layer-diagonal contribution. From figure 1 one can see that in the case of a parent lattice, screening of the 'Kambe structure constants' yields the same screening effects as for the folded three-dimensional reciprocal space structure constants discussed by Szunyogh *et al.* (1994). Furthermore it can be seen from figures 1–3 that (1) the screening results in an exponential decay of the structure constants, (2) the unscreened structure constants decay faster the more negative the value of the energy (at an energy of -1.0 ryd the effect of screening is already very small), (3) the screened structure constants are nearly energy independent, and (4) for the two-dimensional structure constants an optimal screening potential of about 1.0 ryd seems to apply.

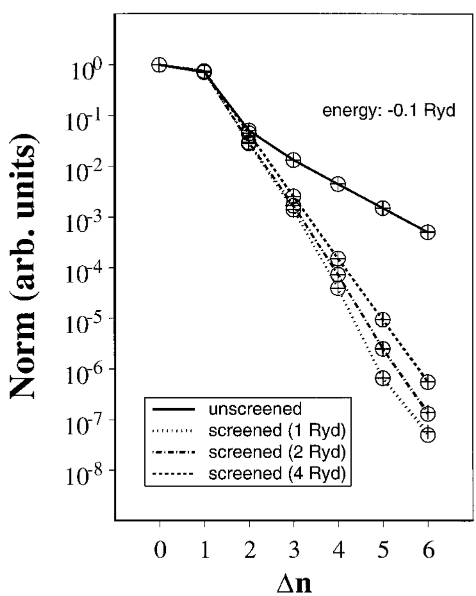

Figure 1. Effect of screening at an energy of -0.1 ryd. For the norm, see equation (12), a logarithmic scale is used. Δn is shown in units of the interlayer spacing. Open circles refer to the 'Kambe structure constants', crosses to folded 3D reciprocal structure constants.

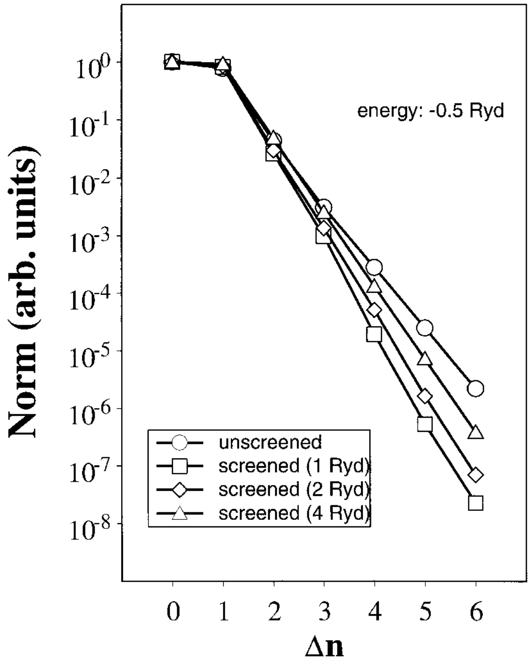

Figure 2. Effect of screening at an energy of − 0.5 ryd. For the norm, see equation (12), a logarithmic scale is used. Δn is shown in units of the interlayer spacing.

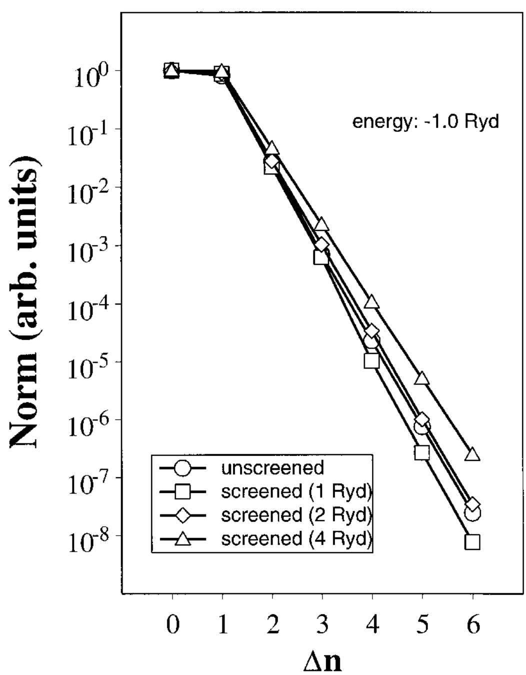

Figure 3. Effect of screening at an energy of − 1.0 ryd. For the norm, see equation (12), a logarithmic scale is used. Δn is shown in units of the interlayer spacing.

It is important to note that the 'Kambe structure constants' are not necessarily restricted to a parent three-dimensional lattice, i.e. in principle the interplane distance can vary from plane to plane, and that they facilitate direct extensions to two-dimensional complex lattices.

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References

Kambe, K., 1967a, *Z. Naturforschung.,* **22a**, 322; 1967b, *Z. Naturforschung.,* **22a**, 422; 1968, *Z. Naturforschung.,* **23a**, 322.

Szunyogh, L., Újfalussy, B., Weinberger, P., and Kollár, J., 1994, *Phys. Rev.,* **B49**, 2721.

Weinberger, P., 1990, *Electron Scattering Theory for Ordered and Disordered Matter* (Oxford: Clarendon Press); 1997, *Phil. Mag.* B, **75**, 509.

Zeller, R., Dederichs, P. H., Újfalussy, B., Szunyogh, L., and Weinberger, P., 1995, *Phys. Rev.,* **B52**, 8807.