On wave propagation
in inhomogeneous systems

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Abstract

We present a theory of electron, electromagnetic, and elastic wave propagation in systems consisting of non-overlapping scatterers in a host medium. The theory provides a framework for a unified description of wave propagation in three-dimensional periodic structures, finite slabs of layered structures, and systems with impurities: isolated impurities, impurity aggregates, or randomly distributed impurities. We point out the similarities and differences between the different cases considered, and discuss the numerical implementation of the formalism.

Key words: Wave propagation; Inhomogeneous systems; Multiple scattering; Photonic crystals; Phononic crystals

1 Introduction

The Korringa-Kohn-Rostoker (KKR) method [1] has been used extensively in the study of the electronic structure and related properties of materials. It has been very successful in calculations of the electronic structure of ordered elemental solids [2], impurities [3], and disordered alloys [4]. Based on the multiple-scattering theory [5], the KKR method calculates from first principles quantities such as the electron density and the ground-state energy of the system. A KKR method for layered systems, the so-called layer KKR (LKKR)
method, has also been developed [6,7]. This method is well adapted to calculations of low-energy electron diffraction (LEED) [8] and electron emission [9] spectra.

In recent years, propagation of classical waves [electromagnetic (EM) or elastic waves] in composite materials with dielectric or, respectively, elastic properties which are periodic functions of the position, with a period comparable to the wavelength of the corresponding field, has been the object of considerable attention [10]. These materials, photonic and phononic crystals, respectively, whether they exist naturally or are artificially fabricated, exhibit a rich variety of physical properties of interest to fundamental and applied research. There are striking analogies between the propagation of electrons in ordinary crystals and EM/elastic waves in photonic/phononic crystals, so that a great variety of multiple-scattering methods originally developed for electronic-structure calculations have been transferred to the field of photonic and phononic crystals [11–15]. The aim of the present article is to present the KKR formalism for electron, EM and elastic waves from a unifying point of view.

2 Multipole expansion of a wave field

We first consider, as an example of a field with one degree of freedom, the case of a spinless particle of mass \( m \) and energy \( \mathcal{E} \), in a potential \( V(\mathbf{r}) \). According to quantum mechanics, the particle is described by a scalar field: the single-particle wave function

\[
\Psi(\mathbf{r}; t) = \Psi(\mathbf{r}) \exp\left(-i\mathcal{E}t/\hbar\right),
\]

where \( \hbar \) is the Planck constant and \( \Psi(\mathbf{r}) \) satisfies the time-independent Schrödinger equation [16]

\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mathcal{E}\right] \Psi = 0 .
\]

In a region of constant potential, \( V_0 \), Eq. (2) reduces to the Helmholtz wave equation

\[
\left[\nabla^2 + q^2\right] \Psi = 0 ,
\]

where \( q = \sqrt{2m(\mathcal{E} - V_0)/\hbar} \). A complete set of spherical-wave solutions of Eq. (3) is given by

\[
\Psi_{\ell m}(\mathbf{r}) = f_\ell(qr)Y^m_\ell(\hat{\mathbf{r}}) ,
\]
where $Y^m_\ell(\hat{\bf r})$ are the usual spherical harmonics and $f_\ell$ may be any linear combination of the spherical Bessel function, $j_\ell$, and the spherical Hankel function, $h_\ell^+$. The most general wave function in a constant potential field can be written as linear sum of the spherical waves given by Eq. (4), as follows:

$$\Psi(\mathbf{r}) = \sum_{\ell m} a_{\ell m} f_\ell(q_\ell \mathbf{r}) Y^m_\ell(\hat{\mathbf{r}}),$$  \hspace{1cm} (5)

where $a_{\ell m}$ are coefficients to be determined.

A vector field has in general, not one, but three degrees of freedom. Let us, for example, consider a harmonic elastic wave, of angular frequency $\omega$, propagating in a homogeneous medium of mass density $\rho$ and Lamé coefficients $\lambda$, $\mu$. This is described by a displacement vector field:

$$\mathbf{U}(\mathbf{r}, t) = \text{Re} \left[ \mathbf{U}(\mathbf{r}) \exp(-i\omega t) \right],$$  \hspace{1cm} (6)

where $\mathbf{U}(\mathbf{r})$ satisfies the equation [17]

$$(\lambda + 2\mu) \nabla (\nabla \cdot \mathbf{U}) - \mu \nabla \times (\nabla \times \mathbf{U}) + \rho \omega^2 \mathbf{U} = 0.$$  \hspace{1cm} (7)

The most general solution of Eq. (7) consists of two types of elastic waves which propagate independently. These are purely longitudinal (irrotational) waves ($\nabla \times \mathbf{U} = 0$), which satisfy the vector Helmholtz equation

$$\left[ \nabla^2 + q^2_L \right] \mathbf{U} = 0,$$  \hspace{1cm} (8)

where $q_L = \omega/c_L$, with $c_L = \sqrt{(\lambda + 2\mu)/\rho}$ being the longitudinal-wave speed; and purely transverse (divergence-free) waves ($\nabla \cdot \mathbf{U} = 0$), which satisfy the vector Helmholtz equation

$$\left[ \nabla^2 + q^2_T \right] \mathbf{U} = 0,$$  \hspace{1cm} (9)

where $q_T = \omega/c_T$, with $c_T = \sqrt{\mu/\rho}$ being the transverse-wave speed. A complete set of longitudinal ($L$) spherical-wave solutions of Eq. (8) is given by [18]

$$\mathbf{U}^L_{\ell m}(\mathbf{r}) = \frac{1}{q_L} \nabla \left[ f_\ell(q_\ell \mathbf{r}) Y^m_\ell(\hat{\mathbf{r}}) \right].$$  \hspace{1cm} (10)

A complete set of transverse ($M, N$) spherical-wave solutions of Eq. (9) is given by [18]

$$\mathbf{U}^M_{\ell m}(\mathbf{r}) = f_\ell(q_\ell \mathbf{r}) \mathbf{X}_{\ell m}(\hat{\mathbf{r}})$$  \hspace{1cm} (11)
\[ U_{\ell m}^N(r) = \frac{i}{q_{\ell}} \nabla \times f_{\ell}(q_{\ell}r) X_{\ell m}(\hat{r}), \quad (12) \]

where \( X_{\ell m}(\hat{r}) \) are the so-called vector spherical harmonics, which are defined by
\[
\sqrt{\ell(\ell + 1)} X_{\ell m}(\hat{r}) = L Y_{\ell m}(\hat{r}) \equiv -i \hat{r} \times \nabla Y_{\ell m}(\hat{r}). \quad (13)\]

The most general displacement field in a homogeneous medium can be written as a linear sum of the spherical waves given by Eqs. (10)-(12), as follows
\[
U(r) = \sum_{\ell m} \left\{ a_{\ell m}^M f_{\ell}(q_{\ell}r) X_{\ell m}(\hat{r}) + \frac{i}{q_{\ell}} a_{\ell m}^N \nabla \times f_{\ell}(q_{\ell}r) X_{\ell m}(\hat{r})
+ \frac{l}{q_{\ell}} a_{\ell m}^L \nabla \left[ f_{\ell}(q_{\ell}r) Y_{\ell m}(\hat{r}) \right] \right\}, \quad (14)\]

where \( a_{\ell m}^P, P = M, N, L, \) are coefficients to be determined.

Another example of a vector field is the EM field. A harmonic EM wave, of angular frequency \( \omega \), is described by its electric-field component
\[
E(r, t) = \text{Re} \left[ E(r) \exp(-i\omega t) \right]. \quad (15)\]

We need not write down explicitly the magnetic-field component of the wave since this can be readily obtained from \( E(r, t) \) using one of Maxwell equations. In a homogeneous medium characterized by a dielectric function \( \epsilon(\omega) \epsilon_0 \) and a magnetic permeability \( \mu(\omega) \mu_0 \), where \( \epsilon_0, \mu_0 \) are the electric permittivity and magnetic permeability of vacuum, Maxwell equations imply that \( E(r) \) satisfies a vector Helmholtz equation, subject to the condition \( \nabla \cdot E = 0 \), with a wave number \( q = \omega/c \), where \( c = 1/\sqrt{\mu \epsilon \mu_0 \epsilon_0} \) is the velocity of light in the medium. The spherical-wave expansion of \( E(r) \) is given by the terms of Eq. (14) which satisfy \( \nabla \cdot E = 0 \), i.e.,
\[
E(r) = \sum_{\ell m} \left\{ a_{\ell m}^H f_{\ell}(q_{\ell}r) X_{\ell m}(\hat{r}) + a_{\ell m}^E \frac{i}{q} \nabla \times [ f_{\ell}(q_{\ell}r) X_{\ell m}(\hat{r}) ] \right\}, \quad (16)\]

where \( a_{\ell m}^P, P = H, E, \) are coefficients to be determined.
3 Scattering by a single scatterer

We consider a scatterer of finite range, $S$, with its center at the origin of coordinates, and assume that the appropriate in each case characteristics (potential, Lamé coefficients and mass density, electric permittivity and magnetic permeability) are different from those of the surrounding homogeneous medium. A De Broglie, EM or an elastic plane wave incident on this scatterer is described, respectively, by Eq. (4), (16) or (14) with $f_\ell = j_\ell$ (since the plane wave is finite everywhere) and appropriate coefficients $a^0_L$, where $L$ denotes collectively the indices $\ell m P$. Similarly, the scattered wave is described by Eq. (4), (16) or (14) with $f_\ell = h^+_\ell$, which has the asymptotic form appropriate to an outgoing spherical wave: $h^+_\ell \approx (-i)^{\ell} \exp(\imath qr)/\imath qr$ as $r \to \infty$, and appropriate expansion coefficients $a^+_L$. The wavefield for $r > S$ is the sum of the incident and scattered waves. The spherical-wave expansion of the field for $r < S$ is obtained in similar manner by the requirement that it be finite at the origin ($r = 0$).

By applying the proper in each case boundary conditions at the surface of the scatterer, we obtain a relation between the expansion coefficients of the incident and the scattered field, as follows:

$$a^+_L = \sum_{L'} T_{LL'} a^0_{L'} ,$$  \hspace{1cm} (17)

where $T_{LL'}$ are the elements of the so-called scattering transition matrix. Eq. (17) is valid for any shape of scatterer; for spherically symmetric scatterers each spherical wave scatters independently of all others, which leads to a transition matrix diagonal in angular momentum. Explicit forms for $T_{LL'}$ for various cases can be found elsewhere [16,19,20].

4 Multiple scattering theory

We consider an assembly of non-overlapping scatterers centered on sites $R_i$ in a homogeneous medium. In general: an outgoing wave about $R'_i$ [described by Eq. (4), (14) or (16) with $f_\ell = h^+_\ell$ and expansion coefficients $b^+_L$] can be expanded into spherical waves about $R_i$, incident on $R'_i$. This expansion has the form of Eq. (4), (14) or (16) with $f_\ell = j_\ell$ and expansion coefficients $b^i_L(\ell')$, given by

$$b^i_L(\ell') = \sum_{L'} \Omega^{i'i'}_{LL'} b^{+i'}_{L'} .$$ \hspace{1cm} (18)

Explicit expressions for the so-called free-space structural Green functions, $\Omega^{i'i'}_{LL'}$, for the scalar and transverse vector fields can be found elsewhere [4,21].
In the case of the elastic field, since a longitudinal (transverse) spherical wave about \( \mathbf{R}_i \) remains a longitudinal (transverse) wave when expanded about another center \( \mathbf{R}_i \neq \mathbf{R}_i' \), the matrix elements \( \Omega_{LL'}^{ii'} \) are obtained independently for longitudinal and transverse waves. Therefore, \( \Omega_{LL'}^{ii'} \) has a block-diagonal form in the mode index \( P \) (we recall that \( L \equiv \ell m P \)): the matrix elements of the block corresponding to transverse waves are identical to the corresponding matrix elements for the EM field, while the matrix elements of the block corresponding to longitudinal waves are identical to the corresponding matrix elements for the scalar field [15]. We note that, for any field, by definition, \( \Omega_{LL'}^{ii'} \) equals zero for \( i = i' \).

The wave scattered from the scatterer at \( \mathbf{R}_i \) is determined from the total wave incident on this scatterer; therefore

\[
b_L^{+i} = \sum_{L'} T_{LL'}^i (a_{L'}^0 + b_{L'}^{ii'}) ,
\]

where \( a_{L'}^0 \) are the coefficients in the multipole expansion [given by Eq. (4), (14) or (16)] about \( \mathbf{R}_i \) of an externally incident wave; and \( b_{L'}^{ii'} \) are the coefficients in the multipole expansion about \( \mathbf{R}_i \) of the outgoing waves scattered from all the other scatterers at \( \mathbf{R}_i \neq \mathbf{R}_i' \). From Eq. (18) we have

\[
b_{L'}^{ii'} = \sum_{i', L'} \Omega_{LL'}^{ii'} b_L^{+i} .
\]

Substituting Eq. (20) into Eq. (19) we obtain

\[
\sum_{i', L'} \left( \delta_{ii'} \delta_{LL'} - \sum_{L''} T_{LL''}^i \Omega_{LL'}^{ii''} T_{L''L'}^{i''} \right) b_{L'}^{+i'} = \sum_{L'} T_{LL'}^i a_{L'}^0 .
\]

We now introduce the structural Green functions \( D_{LL'}^{ii'} \) which give the coefficients [in an expansion such as (4), (14) or (16)] of the wave incident on the scatterer at \( \mathbf{R}_i \), due to an outgoing wave from the scatterer at \( \mathbf{R}_i' \). An outgoing wave from the \( i' \)th scatterer can reach the \( i \)th scatterer directly, or indirectly after scattering any number of times by any number of scatterers (including those at \( \mathbf{R}_i \) and \( \mathbf{R}_i' \)). Let \( D_{LL'}^{ii'} \) express the sum of the contribution to the coefficients of the incident wave on \( \mathbf{R}_i \) from all possible scattering paths originating from an outgoing wave from the \( i' \)th scatterer. One can easily prove by iteration the following equation

\[
D_{LL'}^{ii'} = \Omega_{LL'}^{ii'} + \sum_{i', L'', L'''} \Omega_{LL''}^{ii'} T_{L''L'}^{ii''} D_{L''L'}^{ii'} ,
\]

where \( \delta_{ii'} \) is the Kronecker delta.
where $T^{ii''}_{L''L'''}$ are the elements of the transition matrix which describes the scattering by the single scatterer at $R_i$. We generalize Eq. (22) by treating the scattering at $R_i$ in two stages. The first-stage scattering is described by $T^{ri}_{LL'}$, which correspond to arbitrarily defined scatterers (reference scatterers), and the second-stage scattering by $T^{i}_{LL'} - T^{ri}_{LL'}$. We obtain:

$$D^{ii'}_{LL'} = D^{ri}_{LL'} + \sum_{i',L',L''} D^{ri'}_{LL'} \left( T^{i''}_{L''L'''} - T^{ri'}_{L''L'''} \right) D^{i'i''}_{L''L'''} , \quad (23)$$

where $D^{ri'}_{LL'}$ are the solution of Eq. (22) when $T^{i}_{LL'} = T^{ri}_{LL'}$.

5 Bulk systems

We consider the case in which the scatterers constitute a three dimensional (3D) crystal structure specified by Bravais lattice vectors $R_n$ and non-primitive translation vectors, indicating the positions of the scatterers within the unit cell, $\mathbf{t}_\alpha$; in this case the site index $i$ stands for the composite index $n\alpha$. Bloch’s theorem implies that $b^+_{L'} n\alpha' = \exp [i \mathbf{k} \cdot (R_{n'} - R_n)] b^+_{L'} n\alpha'$. The normal modes of the crystal are obtained, by putting the external incident wave equal to zero in Eq. (21), which leads to the following secular equation:

$$\det \left[ \delta_{\alpha\alpha'} \delta_{LL'} - \sum_{L''} T^{\alpha}_{LL'} \Omega^{\alpha\alpha'}_{L''L'''}(k) \right] = 0 , \quad (24)$$

where

$$\Omega^{\alpha\alpha'}_{LL'}(k) = \sum_{n'} \Omega^{\alpha\alpha' n\alpha'}_{LL'} \exp [i \mathbf{k} \cdot (R_{n'} - R_n)] , \quad (25)$$

which does not depend on $n$. Both $T^{\alpha}_{LL'}$ and $\Omega^{\alpha\alpha'}_{LL'}(k)$ in Eq. (24) are functions of the frequency of the wave, but the $T^{\alpha}_{LL'}$ depend only on the properties of a single scatterer, whereas $\Omega^{\alpha\alpha'}_{LL'}(k)$ depend only on the geometry. Thus Eq. (24) reflects a complete separation of the individual scatterer and structural aspects of the problem. The matrix elements $\Omega^{\alpha\alpha'}_{LL'}(k)$ for the scalar field were introduced by Korringa, Kohn, and Rostoker [1] in relation to the calculation of the electronic band structure of periodic solids and are commonly referred to as the KKR structure constants. The calculation of the structure constants, which needs to be done only once for a given lattice, usually requires Ewald-summation techniques [22]. We note that Eq. (24) involves in principle infinite-dimensional matrices. In actual calculations, however, it is sufficient to truncate the angular momentum index, $\ell$, to some relatively small
number, \( \ell_{\text{max}} \). The KKR method has been successfully used for many years in the calculation of the electron band structure of solids [2], and more recently it has also been applied to the calculation of the frequency band structure of EM and elastic fields in relation to photonic and phononic crystals [14].

One of the advantages of the KKR theory compared to other approaches is its capability of dealing with defects and disorder [4]. For the description of point defects at a finite number of sites, one needs to calculate the structural Green functions, \( D^{ii'}_{LL'} \), of the defect system. This can be done in real space, using Eq. (23) and considering the periodic crystal (without any defect) as the reference system. In this case, the sum over \( i'' \) in Eq. (23) is restricted to those sites at which there are defects and induce a perturbation \( \delta T^{i'n'l''}_{L'n'L''} = T^{i'n'l''}_{L'n'L''} - T^{r'i'n'}_{L'r'L'} \) on the \( T \) matrix. For the periodic arrangement of scatterers of the reference system, the evaluation of \( D^{ri'i'}_{LL'} \) through Eq. (22) involves an infinite number of sites and it is achieved by a lattice Fourier transform of Eq. (22)

\[
D^{\alpha\alpha'}_{LL'}(\mathbf{k}) = \Omega^{\alpha\alpha'}_{LL'}(\mathbf{k}) + \sum_{\alpha'',L'',L'''} \Omega^{\alpha\alpha''}_{LL'''}(\mathbf{k}) T^{r\alpha''}_{L''L'''} D^{\alpha'n''}_{L''L'''}(\mathbf{k}) \tag{26}
\]

and subsequent integration over the volume \( v \) of the Brillouin zone (BZ)

\[
D^{ri'i'}_{LL'} = \frac{1}{v} \int_{\text{BZ}} \exp \left[ i \mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_{n'}) \right] D^{r\alpha\alpha'}_{LL'}(\mathbf{k}) \tag{27}
\]

If a number of \( N \) different scatterers, described by \( T \) matrices \( T^j_{LL'} \), \( j = 1, 2, \ldots, N \), are randomly distributed on the sites of a given crystal, the coherent potential approximation (CPA) [23] can be used to treat the disordered system within a mean-field context. The effective CPA medium consists of identical scatterers at all sites of sublattice \( \alpha \) of the crystal, characterized by a \( T \) matrix \( T^\alpha_{LL'} \). The structural Green functions \( D^{n\alpha'n'\alpha'}_{LL'} \) of the CPA medium are calculated by equations analogous to (26) and (27). The CPA self-consistency condition demands that the correction to the scattering due to the difference of the actual scatterers from the CPA scatterer vanishes on the average

\[
\sum_{j=1}^{N} c_{j;\alpha} \left[ (T^j - T^c_{\alpha}) D^{\alpha\alpha\alpha}_{0\alpha;0\alpha} \right]^{-1} (T^j - T^c_{\alpha}) = 0 \quad \text{for every } \alpha, \tag{28}
\]

where \( c_{j;\alpha} \) denotes the concentration of scatterer \( j \) on sublattice \( \alpha \).
6 Layered systems

A layered system consists of a number of planes (layers) of scatterers with the same two dimensional (2D) periodicity. To begin with, we consider just one layer, at $z = 0$, in which case the scatterers are centered on the sites $\mathbf{R}_n + t_\alpha$, where $\{\mathbf{R}_n\}$ constitutes a 2D Bravais lattice and $t_\alpha$ denote the positions of the scatterers within the 2D unit cell. The 2D reciprocal vectors $\mathbf{g}$, and the surface Brillouin zone (SBZ) corresponding to this lattice are defined in the usual manner [8,9]. The wave vector parallel to the plane of atoms can always be written as follows:

$$\mathbf{q}_\parallel = \mathbf{k}_\parallel + \mathbf{g'},\quad (29)$$

where the reduced wave vector, $\mathbf{k}_\parallel$, lies in the SBZ and $\mathbf{g'}$ is a certain reciprocal vector. In what follows we write the wave vector of a plane wave of given $\mathbf{q}_\parallel = \mathbf{k}_\parallel + \mathbf{g}$ and given wave number $q_\nu$, where $\nu$ specifies the polarization mode of the wave, if there exist longitudinal and transverse modes, as follows:

$$K_{g\nu}^\pm = \left( \mathbf{k}_\parallel + \mathbf{g}, \pm \left[ q_\nu^2 - (\mathbf{k}_\parallel + \mathbf{g})^2 \right]^{1/2} \right).\quad (30)$$

We note that when $q_\nu^2 < (\mathbf{k}_\parallel + \mathbf{g})^2$, the above defines a decaying wave; the positive (negative) sign in Eq. (30) corresponds to a wave propagating or decaying to the right (left).

The coefficients $b_L^{+n\alpha}$ in the multipole expansion of the scattered field from the layer are obtained from Eq. (21). Using the Bloch condition: $b_L^{+n'\alpha'} = \exp\left[ i\mathbf{k}_\parallel \cdot (\mathbf{R}_{n'} - \mathbf{R}_n) \right] b_L^{+n\alpha'}$, we obtain

$$\sum_{\alpha',L'} \left[ \delta_{\alpha\alpha'}^{n\alpha'} + T_{LL'}^{\alpha\alpha'}(\mathbf{k}_\parallel) \right] b_L^{+n\alpha'} = \sum_{L'} T_{LL'}^{\alpha} a_{L'}^{0n\alpha},\quad (31)$$

where $a_{L'}^{0n\alpha}$ are the coefficients in the multipole expansion of the incident plane wave. The 2D KKR structure constants

$$\Omega_{LL'}^{\alpha\alpha'}(\mathbf{k}_\parallel) = \sum_{n'} \Omega_{LL'}^{n\alpha,n'\alpha} \exp\left[ i\mathbf{k}_\parallel \cdot (\mathbf{R}_{n'} - \mathbf{R}_n) \right],\quad (32)$$

like their counterparts in 3D given by Eq. (25), can be evaluated using Ewald-summation techniques [6].

Writing the incident, reflected and transmitted plane waves with respect to an origin (a scattering center) in this plane, we obtain the amplitudes, $[\Phi_{n1}]^\pm_{g_1}$.
and \([\Phi_{\text{tr}}]_{gi}^{\pm}\) of the reflected and transmitted beams, respectively, in terms of the amplitudes, \([\Phi_{\text{in}}]_{g'i'}^{\pm}\), of the incident wave as follows:

\[
[\Phi_{\text{tr}}]_{gi}^s = \sum_{i'} M_{g'i':g'i'}^{s's'} [\Phi_{\text{in}}]_{g'i'}^{s'}
\]

where \(s = +(-)\) specifies a wave traveling or decaying to the positive (negative) \(z\) direction, and \(i\) denotes the components of the wave field. A scalar field (\(\Phi \rightarrow \Psi\)) has just one component \((i = 1)\), the displacement vector of the elastic field (\(\Phi \rightarrow U\)) has three components \((i = 1,2,3)\), while the EM field (\(\Phi \rightarrow E\)), because of its transverse nature, has only two independent components, \(i = 1,2\). Explicit expressions for the transmission/reflection matrix elements \(M_{g'i':g'i'}^{s's'}\) for the scalar, elastic, and EM fields can be found elsewhere [8,9,15,24].

The transmission/reflection matrices for a slab which consists of a stack of layers with the same 2D periodicity parallel to a given plane are obtained from the transmission/reflection matrices of the individual layers in the manner described in Refs. [8,9,15,24]. Knowing the transmission/reflection matrices for the slab we can readily obtain the transmission, reflection, and absorption coefficients of the plane wave of Eq. (30) incident on the slab. The LKKR technique summarized in this section is particularly well adapted to layered systems because the computation time scales linearly to the number of layers in the slab. Moreover, because this method does not require periodicity in the direction perpendicular to the layers, it can easily treat heterostructures, slabs with impurity planes [24–27] or even a random succession of different layers, as long as these have the same 2D periodicity.

The LKKR technique provides also the complex band structure of an infinite crystal, viewed as a succession of layers parallel to a given crystallographic plane [8,9,15,24].

Point defects or a random distribution of point defects in the layers of a slab can also be treated along the lines described in Section 5 [4,21,28].

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