Symmetry properties of the scattering path operator for arbitrary translationally invariant systems

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In order to optimize the efficiency of relativistic band-structure calculations for complex systems, one should take full advantage of the magnetic space-group symmetry. Most important for the description of systems with reduced symmetry using the Korringa-Kohn-Rostoker method of band-structure calculation, a general derivation of magnetic symmetry properties of the scattering path operator both in real and reciprocal space is presented. In a straightforward way, this approach can be used to minimize the section of $\vec{k}$ space to be sampled for two- and three-dimensional numerical Brillouin-zone integration. Practical aspects of an implementation of the very general scheme presented are discussed in detail.

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I. INTRODUCTION

Despite the strong increase of available computing power during the last years, the demand for a quantitative theoretical description of increasingly complex electronic systems such as multilayer and surface layer systems and noncollinear spin structures requires an ultimate optimization of computational methods.[1,2] In order to accomplish this, it is indispensable to fully exploit the space-group symmetry of a given solid-state system. Furthermore, the correct symmetry of the system and its properties such as linear-response coefficients are automatically preserved this way, independently from numerical artifacts. Corresponding symmetry considerations for magnetic solids treated in a non- or scalar-relativistic way require the use of magnetic spin-space groups that have been discussed, for example, in detail by Sandratskii.[3] On the other hand, effects such as the orbital magnetism, magneto-optical properties, or magnetocrystalline anisotropy of magnetically ordered systems can only be described taking into account spin-orbit coupling. This complex situation, which is the central issue of this contribution, leads to a considerable reduction of the symmetry of the system compared to its paramagnetic state. In addition, the remaining symmetry has to be described using not only conventional symmetry operators acting in real space but also so-called magnetic symmetry operators, i.e., antiunitary combinations of space-group operators and time reversal.[4,5]

Systems with reduced symmetry such as complex surface layer systems and point defects are most conveniently described in terms of the single-particle Green's function.[6] Within the widely used Korringa-Kohn-Rostoker Green's-function (KKR GF) method, the most time consuming step is in general the calculation of the scattering path operator using $\vec{k}$-space integration methods.[6] In the past, there have been several efforts to minimize the section of the Brillouin zone to be sampled within a nonrelativistic or relativistic band-structure calculation. However, these were either restricted to a rather heuristic level or to relatively simple bulk systems with specific symmetry.[5,7–9]

In the following, we present a general scheme to derive the magnetic asymmetry properties of the scattering path operator both in real and $\vec{k}$ space. Our method is applicable to complex three-dimensional bulk systems as well as arbitrary two-dimensional layer systems. Furthermore, it allows in a straightforward way to deal with point defects or systems with noncollinear spin structure. An important application of this scheme is to find the minimal section of the Brillouin zone to be sampled within a two- or three-dimensional $\vec{k}$-space integration. For this reason, the scheme can also be exploited within conventional $\vec{k}$-space band-structure methods based on the variational principle.[10]

II. THEORETICAL FRAMEWORK AND TECHNICAL DETAILS

A. Multiple-scattering theory

In this section, the basic formalism of multiple-scattering theory is shortly outlined. Most of the discussion is kept at an algebraic level and applies to the relativistic as well as the nonrelativistic version of this approach. Whenever it is necessary to be specific, we will deal with the more complex relativistic treatment of a magnetic solid in the following.

The primary step for electronic structure calculations on the basis of multiple-scattering theory is the partitioning of the effective crystal potential V into *nonoverlapping* atomic cell potentials V^i:[6]

$$V=\sum_i V^i. \tag{1}$$

From the scattering or t operator t^i corresponding to a single isolated cell potential V^i at site i,[6]

$$t^i=V^i+V^iG^0t^i, \tag{2}$$

and the free-particle Green's function G^0, one can construct the t operator T of the whole crystal by introducing the scattering path or τ operator τ^{ij} via the following definition:[11]

$$T=\sum_{ij} \tau^{ij}. \tag{3}$$

The operator τ^{ij} accounts for all possible scattering events between cells i and j and satisfies the following equations of motion:[6]

$$\tau^{ij} = t^i \delta_{ij} + t^i G^0 \sum_{k \neq i} \tau^{kj} \tag{4}$$

$$= t^i \delta_{ij} + \sum_{k \neq j} \tau^{ik} G^0 t^j. \tag{5}$$

Starting from Eqs. (1)–(5), the single-particle Green's function can be shown to take on the following form in the relativistic real-space spin representation:[12,13]

$$G(\vec{r},\vec{r}',E) = \sum_{\Lambda\Lambda'} Z^i_\Lambda(\vec{r},E)\,\tau^{ij}_{\Lambda\Lambda'}(E)\,Z^{j\times}_{\Lambda'}(\vec{r}',E) - \sum_{\Lambda} \{Z^i_\Lambda(\vec{r},E) J^{i\times}_\Lambda(\vec{r}',E)\Theta(r'-r) + J^i_\Lambda(\vec{r},E) Z^{i\times}_\Lambda(\vec{r}',E)\Theta(r-r')\}\delta_{ij}. \tag{6}$$

In the previous equation, Z^i_Λ and J^i_Λ are the regular and irregular solutions, respectively, for the single-site Dirac equation for the potential well at site *i*. The spin-angular character of these functions is specified by $\Lambda=(\kappa,\mu)$ with κ and μ the relativistic spin-orbit and magnetic quantum numbers, respectively.[14] The additional superscript in Eq. (6) indicates the corresponding associated left-hand side solutions to the Dirac equation.[13] Finally, $\tau^{ij}_{\Lambda\Lambda'}$ is defined in the following way:[6]

$$\tau^{ij}_{\Lambda\Lambda'} = \int_{\Omega^i} d^3r \int_{\Omega^j} d^3r'\, j^\times_\Lambda(p(\vec{r}-\vec{R}^i)) \times \tau^{ij}(\vec{r},\vec{r}')\, j_{\Lambda'}(p(\vec{r}'-\vec{R}^j)), \tag{7}$$

with $j^{(\times)}_\Lambda$ the relativistic (left-hand) spherical Bessel function.[14] The integration volume for $\vec{r}$ and $\vec{r}'$ is confined to the volume $\Omega^{i(j)}$ of the cells *i* and *j*, respectively. The real-space lattice vector $\vec{R}^i$ is associated with the cell *i*.

It is worth noting that there is an alternative representation of the single-particle Green's-function in terms of the so-called structural Green's function matrix $\underline{G}^{ij}$ with the following definition:[15]

$$\underline{G}^{ij} = \underline{t}^{i-1}\underline{\tau}^{ij}\underline{t}^{j-1} - \underline{t}^{i-1}\delta_{ij}, \tag{8}$$

where underlines denote matrices with respect to the basis functions labeled by the quantum numbers $\Lambda=(\kappa,\mu)$ [see Eq. (7)]. Obviously, all symmetry properties of $\underline{t}^i$ and $\underline{\tau}^{ij}$ to be presented below can straightforwardly be transferred to $\underline{G}^{ij}$ via Eq. (8).

For the nonrelativistic case, the real-space spin representation of the crystal Green's function and the *t* and τ matrices are completely analogous to the equations given above.[16] Thus, all further steps that depend on the explicit representation of these quantities will be given only for the more complex situation in which a magnetically ordered system is treated in a relativistic way.

B. Symmetry properties of the τ matrix

Independently from the system under consideration, the numerical cost of the KKR GF is usually dominated by the computer time needed for the calculation of the scattering path operator τ. For systems that possess a nontrivial magnetic point-group symmetry such as bulk or surface layer systems with a certain orientation of the magnetization (see below), the numerical effort can be substantially reduced by exploiting the symmetry relations for τ. Furthermore, by taking these relations into account, one ensures that the system does not leave the subspace of proper symmetry during the self-consistent field result cycle that could otherwise be accidentally provoked by numerical errors. In particular, this means that equivalent atoms, i.e., atoms whose cell potentials are connected to one another by a symmetry operation of the Hamiltonian, keep this property during every step in the calculation. As will be shown in the following, representation-independent symmetry relations for the scattering path operator τ can be derived. These follow immediately from the corresponding symmetry properties of the Hamiltonian *H*. If not otherwise stated, the considerations in this section apply to the nonrelativistic as well as the relativistic case.

If the *unitary* operator *U* belongs to the symmetry group of the Hamiltonian *H* in the Hilbert space of single-particle states, by definition this implies[4]

$$H = UHU^{-1}. \tag{9}$$

For an *antiunitary*-symmetry operator *U*, we have

$$H = UH^\dagger U^{-1}, \tag{10}$$

where $H^\dagger$ denotes the Hermitian adjungated operator associated with the Hamiltonian *H*. Because the relation $H=H^\dagger$ is not required to hold, the presence of a complex potential does not change the following considerations. Any antiunitary-symmetry operator *U* of the system can be decomposed according to:

$$U = U'T \tag{11}$$

with U' a unitary operator and *T* the antiunitary time-reversal operator.[4,5]

The largest symmetry group of *H* is called magnetic space group $\mathcal{M}$ of *H*.[5] To deal with the most complex situations, we include also the nonsymmorphic space groups in our considerations that contain symmetry operations that consist of an operation followed by a nonprimitive translation *P* in real space (screw and glide mirror operations).[17] In the following the operation *U* will tacitly include the nonprimitive translation *P* in the case of a nonsymmorphic space group if it is not explicitly split off by writting *PU*. For the sake of simplicity, we furthermore use the same symbols for the operations in the Hilbert space of single-particle states and the corresponding operators in three-dimensional real space. Operators in real space that correspond to antiunitary operators in Hilbert space implicitly exclude the time reversal operation.

Because the unitary operators form a subgroup $\mathcal{H}$ of $\mathcal{M}$, the latter group can be decomposed in *right cosets* of the unitary operators:[5,18]

$$\mathcal{M}=\mathcal{H}\cup_{k=1,n_A}\mathcal{H}U^k, \tag{12}$$

with n_A the number of antiunitary operators U^k in $\mathcal{M}$. For certain magnetic space groups $\mathcal{M}$, $\mathcal{H}$ is identical to $\mathcal{M}$, i.e., one has the special case $n_A=0$. The more complex and general situation, in which $\mathcal{M}$ contains unitary as well as antiunitary symmetry elements, will be considered in the following. In this case the order n_U of the subgroup $\mathcal{H}$ of unitary elements is half as large as the order n of $\mathcal{M}$, i.e., there are as many unitary as antiunitary elements in $\mathcal{M}$ ($n_U=n_A=n/2$).[19] For that reason it is sufficient to restrict the number of generating anti-unitary elements U^k in Eq. (12) to $n_A^*=1$. In the case of a nonmagnetic system the corresponding restriction reads $n_A^*=0$, because no antiunitary operations have to be considered.

Due to the properties of the free Hamiltonian H^0, the free Green's operator G^0 possesses full $O(3)$ symmetry (the energy dependence of the Green's operators will be suppressed in the following). Furthermore, it is invariant under time reversal:[13]

$$G^0=TG^{0\dagger}T^{-1}. \tag{13}$$

The Dyson equation for the Green's operator G,[20]

$$G=G^0+G^0VG, \tag{14}$$

implies that the symmetry properties of H and G are the same as those of the effective potential V.

The cellular decomposition of the effective potential according to Eq. (1), together with Eqs. (9) and (10), lead to the following relations in terms of the unitary- and antiunitary- (†) symmetry operator PU of H:

$$V=(PU)V^{(\dagger)}(PU)^{-1}, \tag{15}$$

$$\sum_i V^i=\sum_i PUV^{i(\dagger)}(PU)^{-1}. \tag{16}$$

The sets $\{V^i\}$ and $\{PUV^{i(\dagger)}(PU)^{-1}\}$ both contain spatially disjoint potentials that cover the whole space. In the following, we make use of the fact that for atomic each cell i there is a cell i' with

$$V^{i'}=PUV^{i(\dagger)}(PU)^{-1}. \tag{17}$$

Because of the translational symmetry, this implies the following relation between the corresponding position vectors $\vec{R}^i$ and $\vec{R}^{i'}$ of cells i and i', respectively:

$$\vec{R}^{i'}=PU\vec{R}^i. \tag{18}$$

For the single-site t operators t^i, we have from Eq. (2) for *unitary* operators PU

$$\begin{aligned}PUt^i(PU)^{-1}&=PUV^i(PU)^{-1}+PUV^iG^0t^i(PU)^{-1}\\&=PUV^i(PU)^{-1}\\&\quad+PUV^i(PU)^{-1}G^0PUt^i(PU)^{-1}\\&=V^{i'}+V^{i'}G^0PUt^i(PU)^{-1}.\end{aligned} \tag{19}$$

For *antiunitary* operators PU, we have analogously

$$\begin{aligned}&PUt^{i\dagger}(PU)^{-1}\\&=(PUt^i(PU)^{-1})^\dagger\\&=(PUV^i(PU)^{-1}+PUV^iG^0t^i(PU)^{-1})^\dagger\\&=PUV^{i\dagger}(PU)^{-1}+PUt^{i\dagger}(PU)^{-1}G^0PUV^{i\dagger}(PU)^{-1}\\&=V^{i'}+PUt^{i\dagger}(PU)^{-1}G^0V^{i'}\\&=V^{i'}+V^{i'}G^0PUt^{i\dagger}(PU)^{-1}.\end{aligned} \tag{20}$$

In the second step, we use the fact that the product of two antiunitary operators yields a unitary operator.[4] Therefore, the same implicit equations hold for $t^{i'}$ and $PUt^{i(\dagger)}(PU)^{-1}$ and we can identify

$$t^{i'}=PUt^{i(\dagger)}(PU)^{-1}. \tag{21}$$

For the special case of a bulk crystal with three-dimensional translational invariance, it is advantageous to separate the cell index i into an index n for the site $\vec{R}^n$ on the Bravais lattice and an index α to label a basis atom within a unit cell. Thus, we have

$$\vec{R}^i=\vec{R}^n+\vec{\rho}^\alpha. \tag{22}$$

By definition, we may write

$$\begin{aligned}t^i&=t^{n,\alpha},\\\tau^{ij}&=\tau^{nm,\alpha\beta}.\end{aligned} \tag{23}$$

For the corresponding lattice Fourier-transformed τ operator, we have

$$\tau^{\alpha\beta}(\vec{k})=\sum_n \tau^{nm,\alpha\beta}e^{-i\vec{k}(\vec{R}^n-\vec{R}^m)}=\sum_n \tau^{n0,\alpha\beta}e^{-i\vec{k}\vec{R}^n}, \tag{24}$$

with $\vec{k}$ a three-dimensional wave vector. In the last step, translational invariance in three dimensions has been used. Fourier back transformation leads to

$$\tau^{nm,\alpha\beta}=\frac{1}{V_{BZ}}\int_{V_{BZ}}d^3k\,\tau^{\alpha\beta}(\vec{k})e^{i\vec{k}(\vec{R}^n-\vec{R}^m)}, \tag{25}$$

with V_{BZ} the volume of the first Brillouin zone. This common choice for the unit cell of the reciprocal lattice facilitates the application of symmetry properties to be discussed below.

To deal with the Brillouin-zone integral in Eq. (25), it is extremely useful to know the symmetry relation connecting the $\vec{k}$-dependent τ matrices $\underline{\tau}^{\alpha\beta}(\vec{k})$ and $\underline{\tau}^{\alpha'\beta'}(\underline{U}\vec{k})$. Starting from Eqs. (4) and (21), one finds

$$\underline{\tau}^{\alpha'\beta'}(\underline{U}\vec{k})=e^{-i\underline{U}\vec{k}(\vec{R}^\alpha-\vec{R}^\beta)}\underline{U}\;\underline{\tau}^{\alpha\beta}(\vec{k})\underline{U}^{-1} \tag{26}$$

for a *unitary* operation $U\in\mathcal{M}$ and

$$\underline{\tau}^{\alpha'\beta'}(\underline{U}\vec{k})=e^{-i\underline{U}\vec{k}(\vec{R}^\alpha-\vec{R}^\beta)}\underline{U}\;\underline{\tau}^{\beta\alpha T}(-\vec{k})\underline{U}^{-1} \tag{27}$$

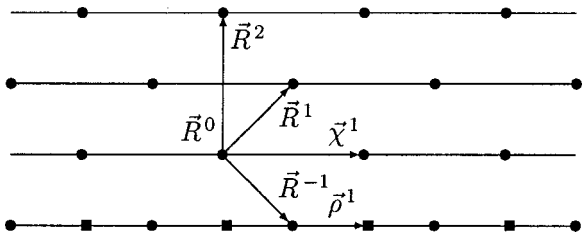

FIG. 1. Orientation of lattice vectors in the layer geometry.

for an *antiunitary* operation $U \in \mathcal{M}$, as it shown in detail in the Appendix. In Eqs. (26) and (27), respectively, $\underline{U}$ denotes the matrix representation of U in real space or spin-angular space, respectively (see the Appendix). $\vec{R}^{\alpha(\beta)}$ are primitive lattice vectors that only depend on the basis atom $\alpha(\beta)$ and the symmetry operation PU.

For an arbitrary layer system, we assume that three-dimensional translational invariance is broken, while two-dimensional translational invariance with respect to the layer plane is preserved. In this case, it is advantageous to separate the cell index i introduced before in a layer index I, an index ν for the part of the lattice vector in the plane, and an index α for the basis atom *in the layer*. While the two-dimensional Bravais lattice specified by the lattice vectors $\vec{\chi}^{\nu}$ is assumed to be the same for all atomic layers, the number and positions of basis atoms may be different in each layer. Thus, we have

$$\vec{R}^i = \vec{R}^I + \vec{\chi}^{\nu} + \vec{\rho}^{\alpha}, \tag{28}$$

with $\vec{R}^I$ the reference vector of the layer I, and $\vec{\rho}^{\alpha}$ the site of a basis atom in layer I (see Fig. 1). The reference vectors $\vec{R}^I$ are usually chosen so as to minimize their norm $|\vec{R}^I|$. By definition, we have

$$t^i = t^{I,\nu,\alpha} \tag{29}$$

and

$$\tau^{ij} = \tau^{IJ,\nu\mu,\alpha\beta}. \tag{30}$$

In analogy to Eq. (24), we define the two-dimensional Fourier transform of the τ matrix with respect to the lattice in the layer plane as

$$\tau^{IJ,\alpha\beta}(\vec{k}_{\parallel}) = \sum_{\nu} \tau^{IJ,\nu\mu,\alpha\beta} e^{-i\vec{k}_{\parallel}(\vec{\chi}^{\nu} - \vec{\chi}^{\mu})}, \tag{31}$$

with $\vec{k}_{\parallel}$ a two-dimensional wave vector. The reverse transformation is accomplished by the two-dimensional Brillouin-zone integral[21]

$$\tau^{IJ,\nu\mu,\alpha\beta} = \frac{1}{A_{BZ}} \int_{A_{BZ}} d^2k \, \tau^{IJ,\alpha\beta}(\vec{k}_{\parallel}) e^{i\vec{k}_{\parallel}(\vec{\chi}^{\nu} - \vec{\chi}^{\mu})}, \tag{32}$$

with A_{BZ} the area of the two-dimensional Brillouin zone of the layer system.

In analogy to Eqs. (26) and (27), one finds for the $\vec{k}$-independent τ matrices $\tau^{IJ,\alpha\beta}(\vec{k}_{\parallel})$ the symmetry relation

$$\underline{\tau}^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_{\parallel}) = e^{i(\underline{U}-\underline{1})\vec{k}_{\parallel}(\vec{R}^I - \vec{R}^J)} \times e^{-i\underline{U}\vec{k}_{\parallel}(\vec{\chi}^{\alpha} - \vec{\chi}^{\beta})} \cdot \underline{U} \, \underline{\tau}^{IJ,\alpha\beta}(\vec{k}_{\parallel}) \underline{U}^{-1} \tag{33}$$

for a *unitary* operator $U \in \mathcal{M}$ and

$$\underline{\tau}^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_{\parallel}) = e^{i(\underline{U}-\underline{1})\vec{k}_{\parallel}(\vec{R}^I - \vec{R}^J)} e^{-i\underline{U}\vec{k}_{\parallel}(\vec{\chi}^{\alpha} - \vec{\chi}^{\beta})} \cdot \underline{U} \, \underline{\tau}^{JI,\beta\alpha T}(-\vec{k}_{\parallel}) \underline{U}^{-1} \tag{34}$$

for an *antiunitary* operator $U \in \mathcal{M}$, with the vectors $\vec{\chi}^{\alpha}$ being primitive lattice vectors that depend only on the positions of the basis atoms α. Concerning the operators U applied to $\vec{k}_{\parallel}$, it is important to note that these are restricted to rotations and mirror operations with their axes or mirror planes oriented perpendicular to the layer plane, respectively.

C. Three- and two-dimensional Brillouin-zone integration

Using Eqs. (26) and (27) and (33) and (34), respectively, the efficiency of three- and two-dimensional Brillouin zone integrations can be greatly improved. In the following, the generating antiunitary operator in the right coset decomposition indicated in Eq. (12) will be denoted by $\tilde{U}$ instead of U for readability. As one can see from Eqs. (27) and (34), the antiunitary operator $\tilde{U}$ in the bispinor space corresponds in the three- or two-dimensional reciprocal space effectively to the operation $I\tilde{U}$ with the inversion I. With the aid of Eq. (12), we can write for the set of orthogonal operators $\mathcal{M}'$ and $\mathcal{H}'$ in reciprocal space that correspond to the groups $\mathcal{M}$ and $\mathcal{H}$, respectively,

$$\mathcal{M}' = \mathcal{H}' \cup_{k=1,\ldots,n_A^*} \mathcal{H}' I \tilde{U}^k. \tag{35}$$

This set represents a group of order n, because of the properties of I:

$$I^{-1} = I, \tag{36}$$

$$\tilde{U}^k I = I \tilde{U}^k$$

for

$$k = 1, \ldots, n_A^*. \tag{37}$$

The symmetry group $\mathcal{S}_{BZ}$ of order n_{BZ} representing the geometrical properties of the reciprocal lattice and the Brillouin zone is identical with the holosymmetric point group of the corresponding crystal system.[22] Because for any three- and two-dimensional translationally invariant lattice the group $\mathcal{S}_{BZ}$ includes the inversion I, the group $\mathcal{M}'$ represents a subgroup of $\mathcal{S}_{BZ}$. Therefore, the following right coset decomposition of $\mathcal{S}_{BZ}$ can be made:

$$\mathcal{S}_{BZ} = \mathcal{M}' \cup_{l=1,\overline{n'_{BZ}}} \mathcal{M}' S_l, \tag{38}$$

where S_l denote those $\overline{n'_{BZ}}$ operators in $\mathcal{S}_{BZ}$ that are not included in $\mathcal{M}'$. As for the decomposition of the magnetic space group $\mathcal{M}$ considered in Eq. (12), there is a minimum

number n'_{BZ} of generating elements S_l for $\mathcal{S}_{BZ}$. This number is obviously given by the relation $n_{BZ}=n(n'_{BZ}+1)$.

The Brillouin zone is covered by application of the n operators in $\mathcal{M}'$ to its so-called irreducible part (IBZ) denoted by V_{IBZ} and A_{IBZ} for three- and two-dimensional systems, respectively. For a nonmagnetic system with one atom per unit cell the group $\mathcal{M}'$ coincides with $\mathcal{S}_{BZ}$ and one therefore has $n'_{BZ}=0$. This situation leads to the smallest possible irreducible part IBZ of the Brillouin zone, which will be denoted by V^*_{IBZ} and A^*_{IBZ}, respectively, in the following. For a magnetic system, the IBZ is obtained by application of the identity $E=S_0$ together with the n'_{BZ} operations S_l on the corresponding Brillouin zone regions V^*_{IBZ} and A^*_{IBZ}, respectively.

Using Eqs. (26) and (27), the three-dimensional Brillouin zone integration in Eq. (25) can be represented in the following way:

$$\begin{aligned}\underline{\tau}^{nm,\alpha'\beta'}&=\frac{1}{V_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{V^*_{IBZ}}d^3k\,\underline{\tau}^{\alpha'\beta'}(\underline{U}^j\underline{S}^l\vec{k})e^{i\underline{U}^j\underline{S}^l\vec{k}(\vec{R}^n-\vec{R}^m)}+\sum_{k=1,\ldots,n^*_A}\underline{\tau}^{\alpha'\beta'}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k})e^{i\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}(\vec{R}^n-\vec{R}^m)}\\&=\frac{1}{V_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{V^*_{IBZ}}d^3k\,\underline{U}^j\underline{\tau}^{\alpha\beta}(\underline{S}^l\vec{k})\underline{U}^{j-1}e^{i\underline{U}^j\underline{S}^l\vec{k}(\vec{R}^n-\vec{R}^m-\vec{R}^\alpha+\vec{R}^\beta)}\\&\quad+\sum_{k=1,\ldots,n^*_A}\underline{U}^j\underline{\tilde{U}}^k\underline{\tau}^{\beta''\alpha''T}(\underline{S}^l\vec{k})\underline{\tilde{U}}^{k-1}\underline{U}^{j-1}e^{i\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}(\vec{R}^n-\vec{R}^m-\vec{R}^{\alpha''}+\vec{R}^{\beta''})}.\end{aligned}\tag{39}$$

The site off-diagonal τ matrix is needed, for instance, for self-consistent calculations of single impurities embedded in a host crystal.[23] For a self-consistent calculation of a crystal system, one is only interested in the site-diagonal elements of the τ matrix, i.e., $n=m$ and $\alpha=\beta$. In this case, Eq. (39) can be further simplified because the exponential factors drop out:

$$\underline{\tau}^{nn,\alpha'\alpha'}=\frac{1}{V_{BZ}}\sum_{j=1,\ldots,n_U}\underline{U}^j\left[\sum_{l=0,\ldots,n'_{BZ}}\left(\int_{V^*_{IBZ}}d^3k\,\underline{\tau}^{\alpha\alpha}(\underline{S}^l\vec{k})+\sum_{k=1,\ldots,n^*_A}\underline{\tilde{U}}^k\int_{V^*_{IBZ}}d^3k\,\underline{\tau}^{\alpha''\alpha''T}(\underline{S}^l\vec{k})\underline{\tilde{U}}^{k-1}\right)\right]\underline{U}^{j-1}.\tag{40}$$

Obviously, the numerical Brillouin-zone integration in the previous equation can be completed *prior to* the multiplication by the matrices $\underline{\tilde{U}}^k$ and $\underline{U}^j$ to save computer time.

For the two-dimensional Brillouin-zone integration in Eq. (32), we have from Eqs. (33) and (34)

$$\begin{aligned}\underline{\tau}^{IJ,\nu\mu,\alpha'\beta'}&=\frac{1}{A_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{A^*_{IBZ}}d^2k\,\underline{\tilde{\tau}}^{IJ,\alpha'\beta'}(\underline{U}^j\underline{S}^l\vec{k}_\parallel)e^{i\underline{U}^j\underline{S}^l\vec{k}_\parallel(\vec{R}^I+\vec{\chi}^\nu-\vec{R}^J-\vec{\chi}^\mu)}\\&\quad+\sum_{k=1,\ldots,n^*_A}\underline{\tilde{\tau}}^{IJ,\alpha'\beta'}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}_\parallel)e^{i\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}_\parallel(\vec{R}^I+\vec{\chi}^\nu-\vec{R}^J-\vec{\chi}^\mu)}\\&=\frac{1}{A_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{A^*_{IBZ}}d^2k\,\underline{U}^j\underline{\tilde{\tau}}^{IJ,\alpha\beta}(\underline{S}^l\vec{k}_\parallel)\underline{U}^{j-1}e^{i\underline{U}^j\underline{S}^l\vec{k}_\parallel(\vec{R}^I+\vec{\chi}^\nu-\vec{R}^J-\vec{\chi}^\mu-\vec{\chi}^\alpha+\vec{\chi}^\beta)}\\&\quad+\sum_{k=1,\ldots,n^*_A}\underline{U}^j\underline{\tilde{U}}^k\underline{\tilde{\tau}}^{JI,\beta''\alpha''T}(\underline{S}^l\vec{k}_\parallel)\underline{\tilde{U}}^{k-1}\underline{U}^{j-1}e^{i\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}_\parallel(\vec{R}^I+\vec{\chi}^\nu-\vec{R}^J-\vec{\chi}^\mu-\vec{\chi}^{\alpha''}+\vec{\chi}^{\beta''})}.\end{aligned}\tag{41}$$

In the previous equation, it is convenient to use the auxiliary quantity $\underline{\tilde{\tau}}^{IJ}$ instead of $\underline{\tau}^{IJ}$:

$$\underline{\tilde{\tau}}^{IJ,\alpha\beta}(\vec{k}_\parallel)=\underline{\tau}^{IJ,\alpha\beta}(\vec{k}_\parallel)e^{i\vec{k}_\parallel(\vec{R}^J-\vec{R}^I)}.\tag{42}$$

Similar to the case of the three-dimensional $\vec{k}$-space integration in Eq. (40), the expression on the right-hand side of the previous equation is greatly simplified in the site-diagonal case:

$$\underline{\tau}^{II,\nu\nu,\alpha'\alpha'}=\frac{1}{A_{BZ}}\sum_{j=1,\ldots,n_U}\underline{U}^j\left[\sum_{l=0,\ldots,n'_{BZ}}\left(\int_{A^*_{IBZ}}d^2k\,\underline{\tilde{\tau}}^{II,\alpha\alpha}(\underline{S}^l\vec{k}_\parallel)+\sum_{k=1,\ldots,n^*_A}\underline{\tilde{U}}^k\int_{A^*_{IBZ}}d^2k\,\underline{\tau}^{II\alpha''\alpha''T}(\underline{S}^l\vec{k}_\parallel)\underline{\tilde{U}}^{k-1}\right)\right]\underline{U}^{j-1}.\tag{43}$$

For the evaluation of electronic properties within the framework of the response theory, one is usually faced with the task of performing Brillouin-zone integrations of products of two or even more τ matrices.[24,25] Also in this case, the symmetry properties of the τ matrix can be exploited to greatly improve the numerical efficiency. In the case of linear-response theory, one finds for a three-dimensional problem

$$\begin{aligned}
&\frac{1}{V_{BZ}}\int_{V_{BZ}} d^3k\,\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\vec{k}) \\
&\quad=\frac{1}{V_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{V^*_{IBZ}} d^3k\,\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j\underline{S}^l\vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j\underline{S}^l\vec{k})+\sum_{k=1,\ldots,n^*_A}\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}) \\
&\quad=\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\frac{1}{V_{BZ}}\int_{V^*_{IBZ}} d^3k\,(\underline{U}^j\underline{\tau}^{\alpha\beta}(\underline{S}^l\vec{k})\underline{U}^{j-1})_{\Lambda\Lambda'}(\underline{U}^j\underline{\tau}^{\beta\alpha}(\underline{S}^l\vec{k})\underline{U}^{j-1})_{\Lambda''\Lambda'''} \\
&\qquad+\sum_{k=1,\ldots,n^*_A}(\underline{U}^j\underline{\tilde{U}}^k\underline{\tau}^{\beta''\alpha''T}(\underline{S}^l\vec{k})\underline{\tilde{U}}^{k-1}\underline{U}^{j-1})_{\Lambda\Lambda'}(\underline{U}^j\underline{\tilde{U}}^k\underline{\tau}^{\alpha''\beta''T}(\underline{S}^l\vec{k})\underline{\tilde{U}}^{k-1}\underline{U}^{j-1})_{\Lambda''\Lambda'''}. \qquad (44)
\end{aligned}$$

For two dimensions, the corresponding expression is

$$\begin{aligned}
&\frac{1}{A_{BZ}}\int_{A_{BZ}} d^2k\,\tilde{\tau}^{IJ,\alpha'\beta'}_{\Lambda\Lambda'}(\vec{k}_\parallel)\,\tilde{\tau}^{JI,\beta'\alpha'}_{\Lambda''\Lambda'''}(\vec{k}_\parallel) \\
&\quad=\frac{1}{A_{BZ}}\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\int_{A^*_{IBZ}} d^2k\,\tilde{\tau}^{IJ,\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j\underline{S}^l\vec{k}_\parallel)\,\tilde{\tau}^{JI,\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j\underline{S}^l\vec{k}_\parallel) \\
&\qquad+\sum_{k=1,\ldots,n^*_A}\tilde{\tau}^{IJ,\alpha'\beta'}_{\Lambda\Lambda'}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}_\parallel)\,\tilde{\tau}^{JI,\beta'\alpha'}_{\Lambda''\Lambda'''}(\underline{U}^j\underline{\tilde{U}}^k\underline{S}^l\vec{k}_\parallel) \\
&\quad=\sum_{j=1,\ldots,n_U}\sum_{l=0,\ldots,n'_{BZ}}\frac{1}{A_{BZ}}\int_{A^*_{IBZ}} d^2k\,(\underline{U}^j\underline{\tilde{\tau}}^{IJ,\alpha\beta}(\underline{S}^l\vec{k}_\parallel)\underline{U}^{j-1})_{\Lambda\Lambda'}(\underline{U}^j\underline{\tilde{\tau}}^{JI,\beta\alpha}(\underline{S}^l\vec{k}_\parallel)\underline{U}^{j-1})_{\Lambda''\Lambda'''} \\
&\qquad+\sum_{k=1,\ldots,n^*_A}(\underline{U}^j\underline{\tilde{U}}^k\underline{\tilde{\tau}}^{JI,\beta''\alpha''T}(\underline{S}^l\vec{k}_\parallel)\underline{\tilde{U}}^{k-1}\underline{U}^{j-1})_{\Lambda\Lambda'}(\underline{U}^j\underline{\tilde{U}}^k\underline{\tilde{\tau}}^{IJ,\alpha''\beta''T}(\underline{S}^l\vec{k}_\parallel)\underline{\tilde{U}}^{k-1}\underline{U}^{j-1})_{\Lambda''\Lambda'''}. \qquad (45)
\end{aligned}$$

III. PRACTICAL ASPECTS

A. Determination of the magnetic space group

With the appropriate formalism at hand, the first step for a numerical implementation of a three- or two-dimensional Brillouin-zone integration method is the determination of the magnetic space group $\mathcal{M}$. In the following, we consider explicitly the case of a relativistic system described by a Dirac Hamiltonian of the following form:

$$H(\vec{r})=\frac{c}{i}\vec{\alpha}\vec{\nabla}+\frac{1}{2}(\beta-1)c^2+V(\vec{r})+\beta\vec{\sigma}\vec{B}_{eff}(\vec{r}), \qquad (46)$$

with the scalar potential V and the effective magnetic field $\vec{B}$ in atomic Rydberg units.[26] The Dirac matrices $\vec{\sigma}$, $\vec{\alpha}$, and β have their conventional form.[14] As implied by the notation for the spin-dependent potential term in Eq. (46), the following scheme is not restricted to collinear spin structures but can be applied to noncollinear ones as well. Furthermore, it can be used in connection with spherical symmetric single-site potential terms (muffin-tin and atomic sphere approximation) but also in the full potential case. In the later case it is implied that the choice for the geometrical shape of an atomic cell does not lower the symmetry.

Using Eqs. (9) and (10) and the explicit representation of inversion and rotation operators in bispinor space,[4] the following relation can be shown:

$$\vec{B}_{eff}(\vec{r})=\pm\det\underline{U}\;\underline{U}\vec{B}_{eff}(\underline{U}^{-1}\vec{r}+\vec{p}), \qquad (47)$$

where $\underline{U}$ here denotes the 3×3 matrix corresponding to the proper or improper rotation contained in a specific unitary- or antiunitary-symmetry operator PU and $\vec{p}$ the nonprimitive translation vector corresponding to the operator P. In the previous equation, $+$ holds for unitary and $-$ for antiunitary operations (see below). For the action of time reversal, we have the simple identity[13]

$$TH(-\vec{B}_{eff})T^{-1}=H(\vec{B}_{eff}). \tag{48}$$

To find the various symmetry operations U in $\mathcal{M}$ for a given three-dimensional periodic system with a fixed atomic and magnetic configuration use can be made of the fact that the magnetic space-group of a crystal is a subgroup of the ordinary space group combined with time reversal T. As a consequence, the strategy to find the magnetic space group operations is very similar as for the nonmagnetic situation. First of all one notes that the possible unitary point operations that may occur have to be elements of the holosymmetric point group of the corresponding crystal system [this is identical to $\mathcal{S}_{BZ}$ in Eq. (38)]. The various holosymmetric point groups, which can be taken, for example, from Table 1.3 in Ref. 22, are a subgroup either of the cubic group O_h or the hexagonal group D_{6h}. The Euler angles (α,β,γ) that correspond to the proper rotations U in O_h and D_{6h} are given in Table 2.1 of Ref. 22. These allow to set up the corresponding transformation matrices $\underline{U}$ in the relativistic Λ representation [see Eq. (4.12) in Ref. 27]. Here one should note that the active convention with fixed rotation axes is used by Bradley and Cracknell,[22] while the active temporary convention is used by Rose.[27] Accordingly, the order of the Euler angles have to be reversed. To get the corresponding 3×3-rotation matrices for real-space operations, one calculates the transformation matrices $\underline{U}$ in the nonrelativistic (l,m_l) representation and transforms the submatrix for $l=l'=1$ from spherical to Cartesian coordinates (Sec. 15 in Ref. 27). The matrices representing improper rotations in O_h and D_{6h}, respectively, are obtained from combinations of the inversion and the various proper rotations. The matrix $\underline{I}$ representing the inversion I is given in the Λ representation by $I_{\Lambda\Lambda'}=(-1)^l\delta_{\Lambda\Lambda'}$. Finally, all matrices representing antiunitary operations are obtained by combinations of time reversal T and the various unitary operations. For the Λ representation the matrix representation of T is given by $T_{\Lambda\Lambda'}=S_\kappa(-1)^{\mu+1/2}\delta_{\mu-\mu'}$ with $S_\kappa=\kappa/|\kappa|$ (see also Ref. 5).

Each of the limited number of point operations U found as described above has to be checked whether it maps the system onto itself, i.e., to be a symmetry operation of the system. Eventually, it has to be combined with a subsequent nonprimitive translation P in the case of a nonsymmorphic space group. For U or PU, respectively, to be a symmetry operation it is allowed to connect only sites $\vec{R}^{i'}=PU\vec{R}^i$ [see Eq. (18)] that are occupied by the same chemical element (for a system with substitutional disorder, the elements occupying these sites as well as their concentration have to be the same). In addition, the orientation $\hat{m}$ of the moments ascribed to the atoms on sites at $\vec{R}^i$ and $\vec{R}^{i'}$, respectively, have to be connected by

$$\hat{m}_{\vec{R}^{i'}}=\pm\det\underline{U}\;\underline{U}\hat{m}_{\vec{R}^i}, \tag{49}$$

as is implied by Eq. (47).

For a system with a collinear spin configuration that has all moments oriented along a common direction $\hat{m}$, this leads to obvious restrictions concerning the possible symmetry operations. Among the unitary operations only rotations and screw operations with their axes parallel to $\hat{m}$ are allowed. All mirror or glide mirror planes have to be perpendicular to $\hat{m}$. In addition, the inversion may occur as a unitary element of $\mathcal{H}$. Concerning the antiunitary-symmetry operations, the rotation and screw axes have to be perpendicular to $\hat{m}$, while mirror and glide mirror planes must be parallel to $\hat{m}$.

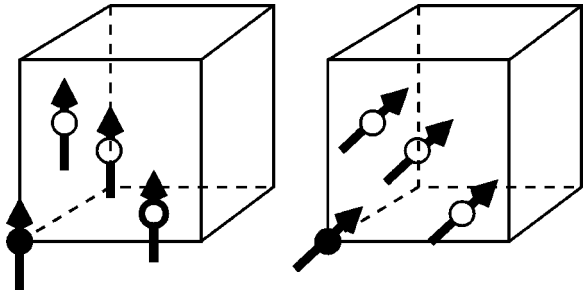

FIG. 2. Equivalent atoms for a system having the Cu_3Au structure and a collinear spin configuration with the magnetic moments pointing along the [001] and [111] axes, respectively.

The restriction in Eq. (49) obviously excludes many operations that might be symmetry operations in the nonmagnetic case. This may cause atoms to be inequivalent that are found to be equivalent when the magnetic configuration is ignored as it is illustrated in Fig. 2 for a system having the Cu_3Au structure. With all magnetic moments pointing along the [001] axis the *white* atom in the basis plane of the cube is inequivalent to the other *white* ones. For the moments pointing along the [111] axis, on the other hand, all *white* atoms are equivalent. The corresponding space-group elements are given in Table I. For further examples, see, e.g., Refs. 5,7, and 28–30.

With the unitary and antiunitary elements of $\mathcal{M}$ determined one can construct the right coset decomposition of $\mathcal{M}$ according to Eq. (12). As has been demonstrated for systems with one atom per unit cell[5] the corresponding generating antiunitary operation U^k can always be chosen to be a twofold rotation $C_{2\perp}$ with its axis perpendicular to $\hat{m}$ followed by time reversal $(U=TC_{2\perp})$. For more complex systems, it also could be a pure nonprimitive translation PE followed by time reversal $(U=TPE)$. For most practical applications, however, using the right coset decomposition of $\mathcal{M}$ doesn't seem to offer much advantages. For that reason the simple decomposition of $\mathcal{M}$ into its subsets of unitary- and antiunitary-symmetry operations $\mathcal{H}$ and $(\mathcal{M}\cap\mathcal{H})$, respectively, is used in the following.

TABLE I. Space-group elements for a system having the Cu_3Au structure with the magnetic moments pointing along the [001] axis and the [111] axis.

$\hat{m}\|[001]$	$E, C_{2z}, C_{4z}^+, C_{4z}^-, I, \sigma_z, S_{4z}^-, S_{4z}^+$
	$TC_{2x}, TC_{2y}, TC_{2a}, TC_{2b}, T\sigma_x, T\sigma_y, T\sigma_{da}, T\sigma_{db}$
$\hat{m}\|[111]$	$E, C_{31}^+, C_{31}^-, I, S_{61}^-, S_{61}^+$
	$TC_{2b}, TC_{2e}, TC_{2f}, T\sigma_{db}, T\sigma_{de}, T\sigma_{df}$

B. Brillouin-zone integration

An application of the symmetry considerations outlined above depend to some extent on the integration scheme used. However, in all cases one has to keep in mind that for antiunitary-symmetry operations the time reversal leads to an additional inversion when dealing with the symmetry properties in reciprocal space [see Eq. (35)]. In the following, the three-dimensional case is considered. The two-dimensional one can be dealt with in an analogous way.

Use of the tetrahedron integration method[31,32] implies that the various matrix elements of the scattering operator matrix τ are stored for the chosen $\vec{k}$ mesh. For that reason it is helpful to find out first which elements have to vanish due to symmetric restrictions. From Eq. (40) one has for the site-diagonal τ matrix

$$\underline{\tau}^{nn,\alpha'\alpha'}_{\Lambda\Lambda'} = \frac{1}{V_{BZ}} \sum_{l=0,\ldots,n'_{BZ}} \int_{V^*_{IBZ}} d^3k \times \sum_{\Lambda''\Lambda'''} \left[\sum_{j=1,\ldots,n_U} U^j_{\Lambda\Lambda''} U^{j*}_{\Lambda'\Lambda'''} \right] \tau^{\alpha\alpha}_{\Lambda''\Lambda'''}(\underline{S}^l\vec{k}) + \left[\sum_{j=1,\ldots,n_A} \tilde{U}^j_{\Lambda\Lambda''} \tilde{U}^{j*}_{\Lambda'\Lambda'''} \right] \tau^{\alpha''\alpha''}_{\Lambda'''\Lambda''}(\underline{S}^l\vec{k}), \quad (50)$$

with the operations S^l creating the irreducible part of the Brillouin zone IBZ out of the associated part with volume V^*_{IBZ}, for which a $\vec{k}$ mesh has to be generated. Obviously, $\tau^{nn,\alpha\alpha}_{\Lambda\Lambda'}$ vanishes if all coefficients in square brackets vanish. For nonvanishing matrix elements, the coefficients may be stored. Because the number of the coefficients get quite large for complex systems or a direction of the magnetization deviating from the global $\hat{z}$ axis, the application of the tetrahedron integration method may be prohibitive.

As an alternative to the tetrahedron integration method, a sampling over a regular mesh of $\vec{k}$ points may be done.[33] In this case a regular mesh spanning the full Brillouin zone is set up first. The number of $\vec{k}$ points is reduced then by keeping only $\vec{k}$ points not connected by a symmetry operation to another one and accounting for a skipped point by increasing the weight of the kept one. In contrast to the nonmagnetic case, the property of an antiunitary operation, as expressed, for example, in Eq. (35), has to be explicitly accounted for when considering the equivalence of two mesh points. This leads finally to the simple expression for the site-diagonal τ matrix

$$\underline{\tau}^{nn,\alpha'\alpha'} = \sum_{j=1,\ldots,n_U} \underline{U}^j \underline{\tau}^{nn,\alpha\alpha}_0 \underline{U}^{j-1} + \sum_{j=1,\ldots,n_A} \underline{\tilde{U}}^j \underline{\tau}^{nn,\alpha''\alpha''T}_0 \underline{\tilde{U}}^{j-1}, \quad (51)$$

with

$$\underline{\tau}^{nn,\alpha\alpha}_0 = \sum_{\vec{k}} w_{\vec{k}} \underline{\tau}^{\alpha\alpha}(\vec{k}). \quad (52)$$

Unfortunately, the situation is less favorable in the case of a calculation of linear-response functions. As implied by Eq. (44), application of the symmetry operations cannot be done after the $\vec{k}$-space integration has been performed. Finding the number of nonvanishing integrals and storing the coefficients for these seems to be more adequate. For the product of two $\vec{k}$-dependent τ matrices to be integrated one has

$$\begin{aligned}\tau^{\alpha'\beta'}_{\Lambda\Lambda'}(\vec{k})\,\tau^{\beta'\alpha'}_{\Lambda''\Lambda'''}(\vec{k}) &= \sum_{\Lambda_a\Lambda_b} \sum_{\Lambda_c\Lambda_d} \left[\sum_{j=1,\ldots,n_U} U^j_{\Lambda\Lambda_a} U^{j*}_{\Lambda'\Lambda_b} U^j_{\Lambda''\Lambda_c} U^{j*}_{\Lambda'''\Lambda_d} \right] \\ &\times \tau^{\alpha\beta}_{\Lambda_a\Lambda_b}(\vec{k})\,\tau^{\beta\alpha}_{\Lambda_c\Lambda_d}(\vec{k}) \\ &+ \left[\sum_{j=1,\ldots,n_A} \tilde{U}^j_{\Lambda\Lambda_a} \tilde{U}^{j*}_{\Lambda'\Lambda_b} \tilde{U}^j_{\Lambda''\Lambda_c} \tilde{U}^{j*}_{\Lambda'''\Lambda_d} \right] \\ &\times \tau^{\beta''\alpha''}_{\Lambda_b\Lambda_a}(\vec{k})\,\tau^{\alpha''\beta''}_{\Lambda_d\Lambda_c}(\vec{k}). \end{aligned} \quad (53)$$

Together with the special point method, this leads to a reasonably good compromise concerning efficiency and storage requirements.

IV. SUMMARY

In order to increase both efficiency and reliability of electronic band-structure calculations using the Green's-function method, we have developed a general method to exploit the magnetic space group symmetry of the scattering path operator. As far as possible, our approach is formulated in terms of abstract operators so as to ensure its applicability both to nonrelativistic and relativistic arbitrary two- and three-dimensional systems. In particular, a systematic and general way to optimize the efficiency of the two- and three-dimensional Brillouin-zone integration is presented. In addition the various practical aspects of an implementation of the approach presented were discussed in detail.

APPENDIX: MAGNETIC SPACE GROUP SYMMETRY AND τ MATRIX

For the scattering path operator τ, from Eqs. (4) and (21) we derive the following relations in terms of the *unitary*-symmetry operator PU of H:

$$\begin{aligned} PU\tau^{ij}(PU)^{-1} &= PUt^i\delta_{ij}(PU)^{-1} + PUt^iG^0\sum_{k\neq i}\tau^{kj}(PU)^{-1} \\ &= t^{i'} + t^{i'}G^0\sum_{k\neq i} PU\tau^{kj}(PU)^{-1} \end{aligned} \quad (A1)$$

and analogously for the *antiunitary* operation PU,

$$
\begin{aligned}
PU\tau^{ji\dagger}(PU)^{-1} &= (PU\tau^{ji}(PU)^{-1})^{\dagger} \\
&= \Bigg(PUt^{j}\delta_{ji}(PU)^{-1} \\
&\quad + PUt^{j}G^{0}\sum_{k\neq j}\tau^{ki}(PU)^{-1}\Bigg)^{\dagger} \\
&= PUt^{i\dagger}\delta_{ij}(PU)^{-1} \\
&\quad + \sum_{k\neq j} PU\tau^{ki\dagger}(PU)^{-1}G^{0}PUt^{j}(PU)^{-1} \\
&= t^{i'}\delta_{i'j'} + \sum_{k\neq j} PU\tau^{ki\dagger}(PU)^{-1}G^{0}t^{j'}.
\end{aligned}
\tag{A2}
$$

Therefore, the same implicit equations hold for $\tau^{i'j'}$ and τ^{ij} or $\tau^{ji\dagger}$, respectively, and we can identify, as in the case of t in Eq. (21),

$$
\tau^{i'j'} = PU\tau^{ij}(PU)^{-1} \tag{A3}
$$

for *unitary* PU and

$$
\tau^{i'j'} = PU\tau^{ji\dagger}(PU)^{-1} \tag{A4}
$$

for *antiunitary* PU.

In the following, we consider explicitly only the unitary or antiunitary magnetic point-group operator U as part of a symmetry operator PU of H while the action of P is implicitly taken into account using Eq. (A5) (see below).

From Eqs. (18) and (22), we derive for the action of PU on $\vec{R}^{i}$

$$
\vec{R}^{i'} = PU\vec{R}^{i} = P(U\vec{R}^{n} + U\vec{\rho}^{\alpha}) = U\vec{R}^{n} + \vec{R}^{\alpha} + \vec{\rho}^{\alpha'} = \vec{R}^{n'} + \vec{\rho}^{\alpha'}, \tag{A5}
$$

where $\vec{R}^{\alpha}$ represents a primitive lattice vector that depends only on α.

For the unitary operator U, we have from Eq. (24)

$$
\begin{aligned}
\tau^{\alpha'\beta'}(\underline{U}\vec{k}) &= \sum_{n} \tau^{nm,\alpha'\beta'} e^{-i\underline{U}\vec{k}(\vec{R}^{n}-\vec{R}^{m})} \\
&= \sum_{n} \tau^{nm,\alpha'\beta'} e^{-i\vec{k}\underline{U}^{-1}(\vec{R}^{n}-\vec{R}^{m})} \\
&= \sum_{n'} \tau^{n'm',\alpha'\beta'} e^{-i\vec{k}(\vec{R}^{n'}-\vec{R}^{m'})} \\
&= e^{-i\underline{U}\vec{k}(\vec{R}^{\alpha}-\vec{R}^{\beta})} PU\tau^{\alpha\beta}(\vec{k})(PU)^{-1},
\end{aligned}
\tag{A6}
$$

where in the last step, use has been made of Eqs. (A3) and (A5). For *anti-unitary U*, we have analogously from Eq. (A4)

$$
\begin{aligned}
\tau^{\alpha'\beta'}(\underline{U}\vec{k}) &= \sum_{n} \tau^{nm,\alpha'\beta'} e^{-i\underline{U}\vec{k}(\vec{R}^{n}-\vec{R}^{m})} \\
&= \sum_{n} \tau^{nm,\alpha'\beta'} e^{-i\vec{k}\underline{U}^{-1}(\vec{R}^{n}-\vec{R}^{m})} \\
&= \sum_{n'} \tau^{n'm',\alpha'\beta'} e^{-i\vec{k}(\vec{R}^{n'}-\vec{R}^{m'})} \\
&= \sum_{n'} PU\tau^{mn,\beta\alpha\dagger}(PU)^{-1} e^{-i\vec{k}\underline{U}^{-1}(\vec{R}^{n'}-\vec{R}^{m'})} \\
&= \sum_{n} PU\tau^{mn,\beta\alpha\dagger} e^{i\vec{k}(\vec{R}^{n}-\vec{R}^{m})}(PU)^{-1} e^{-i\underline{U}\vec{k}(\vec{R}^{\alpha}-\vec{R}^{\beta})} \\
&= e^{-i\underline{U}\vec{k}(\vec{R}^{\alpha}-\vec{R}^{\beta})} PU\tau^{\beta\alpha\dagger}(-\vec{k})(PU)^{-1}.
\end{aligned}
\tag{A7}
$$

In the following, we consider a layer system with two-dimensional translational invariance as introduced in Sec. II A. For the action of the symmetry operation U of the Hamiltonian in real space, we derive in analogy with Eq. (A5)

$$
\begin{aligned}
&PU(\vec{R}^{I} + \vec{\chi}^{\nu} + \vec{\rho}^{\alpha}) \\
&\quad = \underline{U}\vec{R}^{I} + \underline{U}\vec{\chi}^{\nu} + \vec{\chi}^{\alpha} + \vec{\rho}^{\alpha'} = \vec{R}^{I} + \vec{\chi}^{\nu'} + \vec{\rho}^{\alpha'},
\end{aligned}
\tag{A8}
$$

with the primitive in-plane lattice vector $\vec{\chi}^{\alpha}$ that depends only on the basis atom α. For $\vec{\chi}^{\nu'}$, we use the following definition:

$$
\vec{\chi}^{\nu'} = \underline{U}\vec{\chi}^{\nu} + (\underline{U} - \underline{1})\vec{R}^{I} + \vec{\chi}^{\alpha}. \tag{A9}
$$

Let U represent a proper rotation with its axis perpendicular to the layer plane or a mirror operation with the mirror plane perpendicular to the layer plane and P a possible nonprimitive translation parallel to the layer plane.

For *unitary U*, we have from Eqs. (31) and (A3)

$$
\begin{aligned}
\tau^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_{\parallel}) &= \sum_{\nu} \tau^{IJ,\nu\mu,\alpha'\beta'} e^{-i\vec{k}_{\parallel}\underline{U}^{-1}(\vec{\chi}^{\nu}-\vec{\chi}^{\mu})} \\
&= \sum_{\nu'} \tau^{IJ,\nu'\mu',\alpha'\beta'} e^{-i\vec{k}_{\parallel}\underline{U}^{-1}(\vec{\chi}^{\nu'}-\vec{\chi}^{\mu'})} \\
&= e^{i(\underline{U}-\underline{1})\vec{k}_{\parallel}(\vec{R}^{I}-\vec{R}^{J})} e^{-i\underline{U}\vec{k}_{\parallel}(\vec{\chi}^{\alpha}-\vec{\chi}^{\beta})} \\
&\quad \times \sum_{\nu} PU\tau^{IJ,\nu\mu,\alpha\beta}(PU)^{-1} e^{-i\vec{k}_{\parallel}(\vec{\chi}^{\nu}-\vec{\chi}^{\mu})} \\
&= e^{i(\underline{U}-\underline{1})\vec{k}_{\parallel}(\vec{R}^{I}-\vec{R}^{J})} e^{-i\underline{U}\vec{k}_{\parallel}(\vec{\chi}^{\alpha}-\vec{\chi}^{\beta})} PU\tau^{IJ,\alpha\beta}(\vec{k}_{\parallel}) \\
&\quad \times (PU)^{-1},
\end{aligned}
\tag{A10}
$$

where in the second step, use has been made of Eq. (A9). For *antiunitary U*, we have analogously from Eq. (A4)

$$\tau^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_\parallel)=\sum_\nu \tau^{IJ,\nu\mu,\alpha'\beta'}e^{-i\vec{k}_\parallel\underline{U}^{-1}(\vec{\chi}^\nu-\vec{\chi}^\mu)}$$

$$=\sum_{\nu'}\tau^{IJ,\nu'\mu',\alpha'\beta'}e^{-i\vec{k}_\parallel\underline{U}^{-1}(\vec{\chi}^{\nu'}-\vec{\chi}^{\mu'})}$$

$$=e^{i(\underline{U}-1)\vec{k}_\parallel(\vec{R}^I-\vec{R}^J)}e^{-i\underline{U}\vec{k}_\parallel(\vec{\chi}^\alpha-\vec{\chi}^\beta)}$$

$$\times\sum_\nu PU\tau^{JI,\mu\nu,\beta\alpha\dagger}(PU)^{-1}e^{-i\vec{k}_\parallel(\vec{\chi}^\nu-\vec{\chi}^\mu)}$$

$$=e^{i(\underline{U}-1)\vec{k}_\parallel(\vec{R}^I-\vec{R}^J)}e^{-i\underline{U}\vec{k}_\parallel(\vec{\chi}^\alpha-\vec{\chi}^\beta)}PU\tau^{JI,\beta\alpha\dagger}$$

$$\times(-\vec{k}_\parallel)(PU)^{-1}. \tag{A11}$$

In the following, we apply the results concerning symmetry properties of scattering path operators to the special case of the relativistic spin-angular representation.

For the action of the operator U on the regular (left-hand) solutions $j_\Lambda^{(\times)}$, one can show[24,34]

$$\langle\vec{r}|U|j_\Lambda\rangle=\sum_{\Lambda'}U_{\Lambda'\Lambda}j_{\Lambda'}(\vec{r}),$$

$$\langle j_\Lambda^\times|U|\vec{r}\rangle=\sum_{\Lambda'}j_{\Lambda'}^\times(\vec{r})U_{\Lambda\Lambda'}, \tag{A12}$$

with $\underline{U}$ the matrix representation of U. It is important to note that within a specific representation, antiunitary operators can be decomposed uniquely in a unitary part and the operation of complex conjugation.[4] In our formalism, operator matrices $\underline{U}$ in spin-angular space are always to be understood as the representatives of the corresponding *unitary parts* of the operators U.

Using Eq. (7), we have from Eqs. (A3) and (A4)

$$\tau_{\Lambda\Lambda'}^{i'j'}=\int_{\Theta^{i'}}d^3r\int_{\Theta^{j'}}d^3r'\,j_\Lambda^\times(p(\vec{r}-\vec{R}^{i'}))$$

$$\times[PU\tau^{ij}(PU)^{-1}](\vec{r},\vec{r}')j_{\Lambda'}(p(\vec{r}'-\vec{R}^{j'}))$$

$$=\int_{\Theta^i}d^3r\int_{\Theta^j}d^3r'\sum_{\Lambda''\Lambda'''}j_{\Lambda''}^\times(p(\vec{r}-\vec{R}^i))$$

$$\times U_{\Lambda\Lambda''}\tau^{ij}(\vec{r},\vec{r}')U^{-1}_{\Lambda''\Lambda'}j_{\Lambda'''}(p(\vec{r}'-\vec{R}^j))$$

$$=\sum_{\Lambda''\Lambda'''}U_{\Lambda\Lambda''}\tau^{ij}_{\Lambda''\Lambda'''}U^{-1}_{\Lambda''\Lambda'}, \tag{A13}$$

for unitary U and analogously,

$$\tau_{\Lambda\Lambda'}^{i'j'}=\sum_{\Lambda''\Lambda'''}U_{\Lambda\Lambda''}\tau^{jiT}_{\Lambda''\Lambda'''}U^{-1}_{\Lambda''\Lambda'}, \tag{A14}$$

for antiunitary U. As one notes, the nonprimitive translation P does not appear explicitly in the previous two equations. It is rather incorporated in the relation between $\vec{R}^{i(j)}$ and $\vec{R}^{i'(j')}$ according to Eq. (A5).

Using Eqs. (A13) and (A14), Eqs. (A6), (A7), (A10), and (A11) can be formulated in the spin-angular representation

$$\underline{\tau}^{\alpha'\beta'}(\underline{U}\vec{k})=e^{-i\underline{U}\vec{k}(\vec{R}^\alpha-\vec{R}^\beta)}\underline{U}\underline{\tau}^{\alpha\beta}(\vec{k})\underline{U}^{-1}, \tag{A15}$$

$$\underline{\tau}^{\alpha'\beta'}(\underline{U}\vec{k})=e^{-i\underline{U}\vec{k}(\vec{R}^\alpha-\vec{R}^\beta)}\underline{U}\underline{\tau}^{\beta\alpha T}(-\vec{k})\underline{U}^{-1}, \tag{A16}$$

$$\underline{\tau}^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_\parallel)$$

$$=e^{i(\underline{U}-1)\vec{k}_\parallel(\vec{R}^I-\vec{R}^J)}e^{-i\underline{U}\vec{k}_\parallel(\vec{\chi}^\alpha-\vec{\chi}^\beta)}\underline{U}\underline{\tau}^{IJ,\alpha\beta}(\vec{k}_\parallel)\underline{U}^{-1}, \tag{A17}$$

$$\underline{\tau}^{IJ,\alpha'\beta'}(\underline{U}\vec{k}_\parallel)=e^{i(\underline{U}-1)\vec{k}_\parallel(\vec{R}^I-\vec{R}^J)}e^{-i\underline{U}\vec{k}_\parallel(\vec{\chi}^\alpha-\vec{\chi}^\beta)}\underline{U}\underline{\tau}^{JI,\beta\alpha T}$$

$$\times(-\vec{k}_\parallel)\underline{U}^{-1}. \tag{A18}$$

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