

Rotation Matrix Formulation of Tight-binding

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A detailed description of the simplified linear combination of atomic orbitals (LCAO) method implemented within the SO(3) representation is presented.

I. INTRODUCTION

The tight-binding method works by expanding the energy eigenstates of the Hamiltonian in an atomic-like basis set $\{\varphi_{i\alpha}\}$, and replacing the many-body Hamiltonian operator with a parameterized Hamiltonian matrix. In general, the basis set is not explicitly constructed. Nonetheless, it is atomic-like because it has the same symmetry properties as the atomic orbitals. In practice only a small number of basis function are used, those corresponding to the atomic orbitals in the energy range of interest. For instance, when modeling iron only the valence electrons, $3d$ and $4s$, might be considered, while the core electrons can be reasonably neglected since they don't participate in bonding. The energy eigenstates of the system are then obtained by solving the time-independent Schrödinger equation (TISE).

In order to turn an electronic structure method into an atomistic method, total energy and atomic forces are required. The total band energy of a crystal is evaluated by integrating the density of states, $n(\varepsilon)$,

$$E_{\text{band}} = \int_0^{\varepsilon_F} d\varepsilon n(\varepsilon)\varepsilon \quad (1)$$

where ε_F is the Fermi level. The method used to obtain E_{band} , and its derivatives is the difference between the variety of tight-binding methods. All other parts of the energy are typically described by a pairwise potential,

$$E_{\text{repulsive}} = \sum_{i \neq j} U_{ij} \quad (2)$$

where the indices i, j typically run over the atoms in the crystal.

This paper consists of two main parts. In Section II, provides a detailed explanation of the Slater-Koster scheme for tight-binding. The rotation matrix formulation of tight-binding is presented and then explicitly worked out for the case of p -orbitals in Section III. When appropriate, detailed proofs of subtle calculations are provided in the Appendixes. For a recent review article on tight-binding method, the reader is referred to article by Goringe *et. al.*¹

II. SLATER-KOSTER SCHEME FOR TIGHT-BINDING

The starting point for any discussion of the tight-binding method is the Slater and Koster original paper.² The first three sections of the paper are essential reading for anyone with serious interest in the subject. The problem is to find the electronic structure of an extended system. Bloch provided the formal mechanism for dealing with periodic systems, such as crystals by means of the Bloch sum. Starting with an atomic orbital, $\varphi_{i\alpha}(\vec{r} - \vec{R}_i)$, located on atom \vec{R}_i , the Bloch sum is taken over all the periodic images of this orbital,

$$N^{-1/2} \sum_{\vec{n}} \exp(i\vec{k} \cdot \vec{T}_{\vec{n}}) \varphi(\vec{r} - \vec{R}_i - \vec{T}_{\vec{n}}) \quad (3)$$

where N is the number of periodic images, $\vec{T}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ is the translation vector for the lattice, and $\{n_i\} \in \mathbb{Z}$. A proof that Eq. 3 satisfies the Bloch theorem is presented in Appendix A. However, a less explicit notation is used for convenience in the rest of this work,

$$N^{-1/2} \sum_{\vec{R}_i} e^{i\vec{k} \cdot \vec{R}_i} \varphi_{i\alpha}(\vec{r} - \vec{R}_i). \quad (4)$$

Where it is understood that the sum $\sum_{\vec{R}_i}$ is extended over the atoms in equivalent positions \vec{R}_i in all N unit cells of the crystal. In general, it will be necessary to setup such Bloch sums for each atomic orbital (labeled with the Greek character) on each atomic site (labeled with the Roman character) in the periodic-unit cell.

The atomic orbitals, $\varphi_{i\alpha}(\vec{r} - \vec{R}_i)$, are not ideal for the purpose because orbitals on different atomic sites are not orthogonal to one another. Löwdin provided a scheme for creating an orthogonal set from a non-orthogonal one while preserving the symmetry properties of the original set.³ Löwdin function are defined by

$$\psi_{i\alpha} = \sum_{j\beta} S_{i\alpha j\beta}^{-1/2} \varphi_{j\beta} \quad (5)$$

where S is the overlap matrix,

$$S_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} \int d^3r \varphi_{i\alpha}^*(\vec{r} - \vec{R}_i) \varphi_{j\beta}(\vec{r} - \vec{R}_j). \quad (6)$$

The Löwdin construction (Eq. 5) involves evaluating the the reciprocal square root of the overlap matrix. Formally, this is computed by introducing the parameter $\delta S = S - \mathbb{1}$, and expanding with the binomial theorem

$$\begin{aligned} S^{-1/2} &= (\mathbb{1} + \delta S)^{-1/2} \\ &= \mathbb{1} - \frac{1}{2}\delta S + \frac{3}{8}(\delta S)^2 - \frac{5}{16}(\delta S)^3 + \dots, \end{aligned} \quad (7)$$

where $\mathbb{1}$ is the unit matrix.⁷

The Löwdin functions have a greater spatial extent than atomic orbitals, hence the Hamiltonian matrix H will have non-zero matrix elements between atoms with second- or third-nearest neighbors. In the Slater-Koster scheme, Bloch sums are formed from these Löwdin functions, $\psi_{i\alpha}(\vec{r} - \vec{R}_i)$ which are orthonormal.

$$\int d^3r \psi_{i\alpha}^*(\vec{r} - \vec{R}_i) \psi_{j\beta}(\vec{r} - \vec{R}_j) = \delta_{ij}. \quad (8)$$

The Hamiltonian matrix elements are evaluated as a function of \vec{k} with respect to these set of basis function,

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \frac{1}{N} \sum_{\vec{R}_i, \vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} \int d^3r \psi_{i\alpha}^*(\vec{r} - \vec{R}_i) \mathcal{H} \psi_{j\beta}(\vec{r} - \vec{R}_j). \quad (9)$$

This sum simplifies because one of the two sums can be canceled with the factor N^{-1} , giving a sum over the periodic images of one of the two atomic sites,

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} \int d^3r \psi_{i\alpha}^*(\vec{r} - \vec{R}_i) \mathcal{H} \psi_{j\beta}(\vec{r} - \vec{R}_j). \quad (10)$$

Given the Hamiltonian matrix as a function of the wave vector \vec{k} , the band energies $\varepsilon_n(\vec{k})$ are obtained by solving the single-particle TISE,

$$\sum_{j\beta} \mathcal{H}_{i\alpha j\beta}(\vec{k}) c_{n j\beta}(\vec{k}) = \varepsilon_n(\vec{k}) c_{n i\alpha}(\vec{k}), \quad (11)$$

where the $c_{n i\alpha}$ are the expansion coefficients for the Löwdin functions where n is the band index.

The actual calculation of the integrals present in the Hamiltonian matrix is non-trivial. First, we must construct the orthogonalized Löwdin functions from the atomic orbitals. Since the one-electron Hamiltonian,

$$\mathcal{H} = -\frac{\hbar^2}{2m_e} \nabla_{\vec{r}}^2 + \sum_i V(|\vec{r} - \vec{R}_i|), \quad (12)$$

involves a sum of spherically symmetric potentials located at *all* the atoms in the crystal. The integrals involving the periodic potentials in Eq. 10 are classified into four categories:

1. On-site integral - The potential and both orbitals are centered on the same atomic site.
2. Two-center integral - The potential and one orbital is centered on the same atomic site, while the other orbital is at a different location.

3. Three-center integral - The potential and orbitals are all centered on different atomic sites.
4. The fourth category occurs when the orbitals are on the same atomic sites, but the potential is on different atom. This category shares features with both the two-center and three-center integral but is actually a local-environment correction to the on-site terms. This category was ignored by Slater-Koster, but the formalism was later developed by Mercer and Chou.⁴

In the two-center approximation, the only part of the potential energy that we retain is the sum of spherical potentials located on the two atoms on which the atomic orbitals are located. The integral now depends only upon the form of the Löwdin functions, which have the same symmetry as the corresponding atomic orbitals, and the vector between the atoms. The Hamiltonian matrix elements can therefore be written as

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j-\vec{R}_i)} \int d^3r \psi_{i\alpha}^*(\vec{r}-\vec{R}_i) \mathcal{H}_{2c} \psi_{j\beta}(\vec{r}-\vec{R}_j) \quad (13)$$

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j-\vec{R}_i)} F_{\alpha\beta}(R_{ij}) K_{\alpha\beta}(k, l, m) \quad (14)$$

where \mathcal{H}_{2c} is the Hamiltonian within the two-center approximation. The matrix elements in Eq. 14 consists of $F_{\alpha\beta}$ which only depends on the interatomic distance $R_{ij} = |\vec{R}_i - \vec{R}_j|$ and $K_{\alpha\beta}$ which contains the angular dependence on the direction cosines (k, l, m) as taken from Table 1 of Slater and Koster.² (Note that a summation is not implied over repeated indices on the right-hand side of Eq. 14.)

It should be noted that many writers on this problem have assumed that three-center integrals are negligible compared to two-center integrals. This is not necessarily the case, however they are certainly smaller than the two-center integrals. If we regard the tight-binding method as an interpolation scheme rather than an *ab initio* electronic structure method, then the two-center approximation is sufficient, provided we have enough arbitrary constants to fit the information at hand.

The approximations made in the standard forms of orthogonal tight-binding can be summarized as follows:

1. The total energy is divided into the sum of single-electron band energies plus the sum of pair potentials.
2. The Hamiltonian matrix elements are taken to depend only upon the vector between two atoms (two-center approximation).
3. A set of orthogonal basis functions is assumed to exist.
4. Self-consistency is neglected.

III. CALCULATION OF THE p -BAND HAMILTONIAN MATRIX ELEMENTS

The physical interpretation of the $F_{\alpha\beta}$ and $K_{\alpha\beta}$ in Eq. 14 is straightforward if we work in the L_z basis. Consider any two p -orbitals $\alpha = (1, m)$ and $\beta = (1, m')$ on atomic sites (i, j) lying along a common z -axis. This so-called *standard configuration* is depicted in Figure 1. Then by cylindrical symmetry, the Slater-Koster matrix is diagonal.⁸

$$K = \begin{pmatrix} pp\pi & 0 & 0 \\ 0 & pp\sigma & 0 \\ 0 & 0 & pp\pi \end{pmatrix} \quad (15)$$

Appendix B provides a rigorous proof that the Slater-Koster matrix K is diagonal in the quantum numbers (m, m') . There is freedom in our choice for the functional form of $F_{\alpha\beta}(R_{ij})$ in Eq. 14, for simplicity we choose

$$F_{\alpha\beta} = e^{-qR_{ij}}, \quad (16)$$

where q is an *ab initio* fitting parameter.

When the p -orbitals (α, β) lie on atoms (i, j) sharing a common z -axis, we have

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j-\vec{R}_i)} \int d^3r \psi_{i\alpha}^*(\vec{r}-R_i\hat{z}) \mathcal{H}_{2c} \psi_{j\beta}(\vec{r}-R_j\hat{z}) \quad (17)$$

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j-\vec{R}_i)} e^{-qR_{ij}} K_{\alpha\beta}. \quad (18)$$

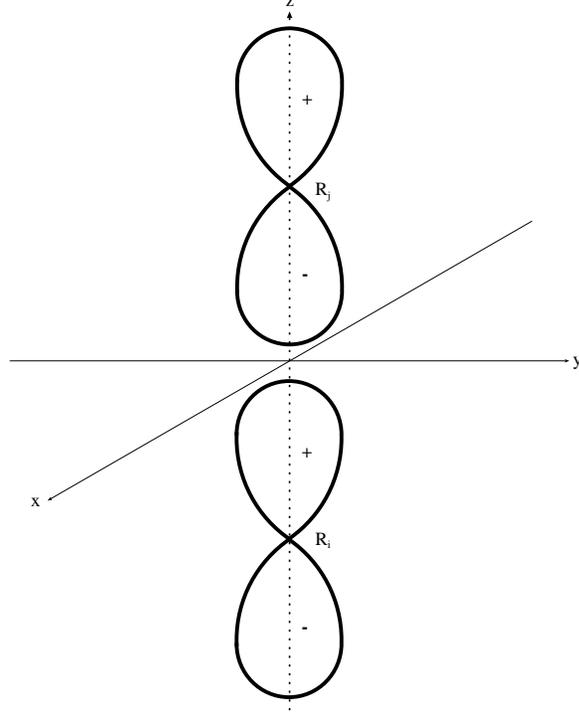


FIG. 1: Two p_z orbitals on atoms (i, j) which lie along the z -axis.

Consider the more general case of two p -orbitals which do *not* lie along a common z -axis. The main idea is to transform the atomic configuration depicted in Figure 2 into the previous case which we already know how to solve. *Both* of the p -orbitals must be rotated so that z' is the new quantization axis.

This turns out to be straightforward by using rotation operators. The generalization of Eq. 18 is

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} \int d^3r \psi_{i\alpha}^*(\vec{r} - \vec{R}_i) \mathcal{H}_{2c} \psi_{j\beta}(\vec{r} - \vec{R}_j) \quad (19)$$

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} e^{-qR_{ij}} \langle \alpha | e^{i\phi_{ij}\hat{L}_z} e^{i\theta_{ij}\hat{L}_y} K e^{-i\theta_{ij}\hat{L}_y} e^{-i\phi_{ij}\hat{L}_z} | \beta \rangle \quad (20)$$

where the angles are defined implicitly through the equation

$$\vec{R}_i - \vec{R}_j = R_{ij} [\sin \theta_{ij} (\hat{x} \cos \phi_{ij} + \hat{y} \sin \phi_{ij}) + \hat{z} \cos \theta_{ij}]. \quad (21)$$

In the L_z representation, the only non-diagonal matrix remaining in Eq. 20 is L_y , which can be explicitly calculated from the lower-raising operators⁵

$$\langle l, m | \hat{L}_y | l', m' \rangle = \frac{1}{2i} \delta_{ll'} \left[\sqrt{l(l+1) - m'(m'+1)} \delta_{m, m'+1} - \sqrt{l(l+1) - m(m-1)} \delta_{m, m'-1} \right] \quad (22)$$

Note that By working in the L_z basis our task has simplified tremendously. However, we want to avoid explicitly calculating the exponential of the non-diagonal matrix $e^{\pm i\theta_{ij}L_y}$, since this involves a power series expansion of the matrix L_y . The standard trick for dealing with this issue is to use a similarity transformation. The L_z representation of the \hat{L}_y operator can be written as

$$\hat{L}_y \doteq M_y L_z M_y^\dagger. \quad (23)$$

where M_y is a matrix whose columns are the eigenstates of the L_y operator written in the L_z basis.

Using Eq. 20, Eq. 23, and the identity $e^{VAV^\dagger} = V e^{AV} V^\dagger$ where V is unitary, the resulting Hamiltonian matrix element in the Slater-Koster scheme is

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} e^{-qR_{ij}} \vec{\alpha}^\dagger e^{i\phi_{ij}L_z} M_y e^{i\theta_{ij}L_z} M_y^\dagger K M_y e^{-i\theta_{ij}L_z} M_y^\dagger e^{-i\phi_{ij}L_z} \vec{\beta}, \quad (24)$$

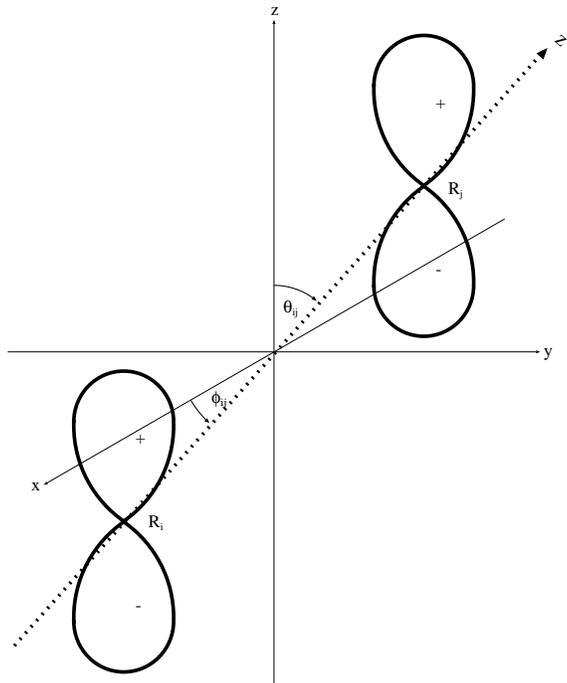


FIG. 2: Two p_z orbitals on atoms (i, j) which *do not* lie along the z -axis.

where α and β are the L_z representation of the orbitals. Typically, these will either be the spherical harmonics or the real orbitals (e.g. p_x, p_y, p_z). The former case is trivial to evaluate because $\vec{\alpha}$ and $\vec{\beta}$ are unit vectors. Using real orbitals, is slightly more complicated and is discussed in Appendix C.

For convenience we introduce the diagonal matrices

$$\Phi_{ij} = \begin{pmatrix} e^{i\phi_{ij}} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\phi_{ij}} \end{pmatrix} \quad (25)$$

and

$$\Theta_{ij} = \begin{pmatrix} e^{i\theta_{ij}} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta_{ij}} \end{pmatrix}. \quad (26)$$

As well as the transformation matrix

$$U_{ij} = M_y \Theta_{ij} M_y^\dagger \Phi_{ij} \quad (27)$$

In terms of these the diagonal matrices, Eq. 24 is given by

$$\mathcal{H}_{i\alpha j\beta}(\vec{k}) = \sum_{\vec{R}_j} e^{i\vec{k}\cdot(\vec{R}_j - \vec{R}_i)} e^{-qR_{ij}} \vec{\alpha}^\dagger U_{ij}^\dagger K U_{ij} \vec{\beta} \quad (28)$$

Table 1 from the Slater and Koster paper can be reproduced by evaluating Eq. 28 for the case of real orbitals. For arbitrary angular momenta, implementing Eq. 24 is straightforward since most of the matrices are diagonal. The most difficult part is calculating the similarity transformation M_y . This is typically accomplished by explicitly constructing L_y as given by Eq.22 and then calling the LAPACK routine **ZHBEV** which diagonalizes band-Hermitian matrices. Note that K is only diagonal in the quantum number m and not ℓ . There are non-zero matrix elements for $\ell \neq \ell'$ and $m = m'$ which obey the rule $\ell\ell'm = (-1)^{\ell+\ell'}(\ell'\ell m)$. For example, the K matrix for spd hybrid orbitals is the

9 × 9 matrix

$$K = \begin{pmatrix} ss\sigma & 0 & -sp\sigma & 0 & 0 & 0 & sd\sigma & 0 & 0 \\ 0 & pp\pi & 0 & 0 & 0 & -pd\pi & 0 & -pd\pi & 0 \\ sp\sigma & 0 & pp\sigma & 0 & 0 & 0 & -pd\sigma & 0 & 0 \\ 0 & 0 & 0 & pp\pi & 0 & -pd\pi & 0 & -pd\pi & 0 \\ 0 & 0 & 0 & 0 & dd\delta & 0 & 0 & 0 & 0 \\ 0 & pd\pi & 0 & pd\pi & 0 & dd\pi & 0 & 0 & 0 \\ sd\sigma & 0 & pd\sigma & 0 & 0 & 0 & dd\sigma & 0 & 0 \\ 0 & pd\pi & 0 & pd\pi & 0 & 0 & 0 & dd\pi & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & dd\delta \end{pmatrix}. \quad (29)$$

APPENDIX A: ATOMIC ORBITAL BLOCH SUM

Bloch's theorem states that the solutions to the TISE for a periodic potential have the special form

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) \quad (A1)$$

where $u_{\vec{k}}(\vec{r})$ has the periodicity of the crystal lattice.

$$u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{T}) \quad (A2)$$

Note that Eq. A1-A2 imply that

$$\psi_{\vec{k}}(\vec{r} + \vec{T}) = e^{i\vec{k}\cdot\vec{T}} \psi_{\vec{k}}(\vec{r}) \quad (A3)$$

for every \vec{T} in the Bravais lattice.

Let explicitly show that

$$\chi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_i} e^{i\vec{k}\cdot\vec{R}_i} \varphi(\vec{r} - \vec{R}_i) \quad (A4)$$

satisfies the Bloch condition Eq. A3.

Consider a translation \vec{T} connecting two lattice points:

$$\chi_{\vec{k}}(\vec{r} + \vec{T}) = \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}_i} \sum_{\vec{R}_i} \varphi(\vec{r} + \vec{T} - \vec{R}_i) \quad (A5)$$

$$= e^{i\vec{k}\cdot\vec{T}} \frac{1}{\sqrt{N}} \sum_{\vec{R}_i} e^{i\vec{k}\cdot(\vec{R}_i - \vec{T})} \varphi(\vec{r} - (\vec{R}_i - \vec{T})) \quad (A6)$$

$$= e^{i\vec{k}\cdot\vec{T}} \chi_{\vec{k}}(\vec{r}) \quad (A7)$$

APPENDIX B: K IS A BLOCK DIAGONAL MATRIX

Although it is a straight forward matter to prove that K is block diagonal in the quantum numbers (m, m') when the basis functions are atomic orbitals, this is not case with the Löwdin functions. In fact, Slater and Koster point this only an approximation on p. 1503 of their paper²

“Actually, the ψ 's are not atomic orbitals, but rather the Löwdin orthogonalized functions, but we have seen that they still have the same symmetry properties with respect to the crystal as the atomic orbitals, and it is not a bad approximation to assume that they can be expanded in the same way. In the integral (2), we shall get nonvanishing components only if we are dealing with σ components of both ψ_n and ψ_m , or π_+ components of both, or π_- components of both, etc.”

Consider the situation depicted in Fig. 1. The Hamiltonian matrix elements within the two-center approximation involve kinetic as well as potential energy integrals.

The potential energy part of the two-center integral in Eq. 13 is given by

$$\int d^3r \varphi_{i\alpha}^*(\vec{r} - \vec{R}_i) V(|\vec{r} - \vec{R}_i|) \varphi_{j\beta}(\vec{r} - \vec{R}_j). \quad (\text{B1})$$

By introducing $\vec{u} \equiv \vec{R}_j - \vec{R}_i$ and using translational invariance, we may write

$$\int d^3r \varphi_{i\alpha}^*(\vec{r}) V(r) \varphi_{j\beta}(\vec{r} - u\hat{z}). \quad (\text{B2})$$

The Slater-Koster matrix K involves the matrix elements between orbitals $\alpha = (n, l, m)$ and $\beta = (n', l', m')$. The two-center integrals of interest are

$$\int d^3r R_{nl}(r) Y_{lm}^*(\theta, \phi) V(r) R_{n'l'}(r') Y_{l'm'}(\theta', \phi') \quad (\text{B3})$$

where $R_{nl}(r)$ is the radial wave functions, $Y_{lm}(\theta, \phi)$ are the spherical harmonics, and n is the principal quantum number.

The primed coordinates (r', θ', ϕ') are spherical coordinates centered on atom j (refer to Fig. 3). The relationship between the prime and unprimed coordinates are:

$$r' = \sqrt{r^2 + u^2 - 2ur \cos \theta} \quad (\text{B4})$$

$$\phi' = \phi \quad (\text{B5})$$

$$\theta' = \pi - \arcsin \left(\frac{r \sin \theta}{\sqrt{r^2 + u^2 - 2ur \cos \theta}} \right). \quad (\text{B6})$$

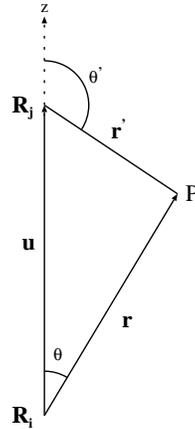


FIG. 3: Two center integration coordinates.

From Eq. B3 and Eq. B5, it follows that the off-diagonal matrix elements of K vanish due to integrals of the form⁹

$$\int d\phi e^{-i(m-m')\phi} = \delta_{mm'} \quad (\text{B7})$$

APPENDIX C: SPHERICAL HARMONIC EXPANSION OF THE REAL ORBITALS

In many electronic structure applications, spherical harmonics prove to be an inconvenient basis. For example, in most crystalline solids spherical symmetry is broken, and azimuthal quantum number m is simply a bad quantum number. Real orbitals are often the basis of choice. Following Sharma's discussion, if the orbitals ψ_α and ψ_β are real, then their angular parts can be of three types,

1. Y_{l0}
2. $\frac{1}{\sqrt{2}} (Y_{l-m} + (-1)^m Y_{lm})$
3. $\frac{i}{\sqrt{2}} (Y_{l-m} - (-1)^m Y_{lm})$

where m is a positive integer.⁶

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⁷ In Löwdin's original paper, δS is defined to be the overlap matrix.

⁸ In this example, K is a 3×3 matrix because $2\ell + 1 = 3$ for p -band orbitals. For treating unhybridized s , p , d orbitals, K would be a 9×9 diagonal matrix. Intuitively, hybridization between orbitals can be introduced by adding off-diagonal terms in K .

⁹ The kinetic energy integrals $\int d^3 r \varphi_{i\alpha}^*(\vec{r} - \vec{R}_i) \left(-\frac{\hbar^2}{2m_e} \nabla_{\vec{r}}^2 \right) \varphi_{j\beta}(\vec{r} - \vec{R}_j)$ vanish for the same reason.