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A DIMENSIONLESS RECIPROCAL LATTICE

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ABSTRACT

The reciprocal lattice vectors widely used in solid state physcis have dimensions of inverse of length and hence will be different in different systems of units. A modified lattice, cross lattice, is defined in such a way that the cross lattice vectors are independent of the coordinate system chosen. Angular momentum eigenfunctions for cross lattice are also obtained.

Introduction

The concept of reciprocal lattice (Kittel, 1976) and the related eigenfunctions play a significant role in the electron theory of solids. Since the reciprocal lattice has dimensions of (length)$^{-1}$, the calculations involving this formulation are dependent on the coordinate system used. A coordinate independent representation could be convenient for comparison purposes. A composition lattice formed from the unit vectors of the direct lattice and the reciprocal lattice could be dimensionless. In this paper we describe such a lattice and obtain the eigenfunctions similar to the momentum eignfunctions used in solid state theory.

The Reciprocal Lattice

Let $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, be the base vectors for ordinary latice. Any vector **L** may, therefore, be represented as (Kittel, 1976)

(1) $\quad \mathbf{L} = L_k \mathbf{a}_k : k = 1, 2, 3$

where repeated indices denote summation according to Einstein convention. L_1, L_2, L_3 are the components of **L** along $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ respectively. The reciprocal lattice vectors for a non-rectangular lattice may be constructed if we take

(2) $\quad \mathbf{b}_k = \epsilon_{klm} (\mathbf{a}_l \times \mathbf{a}_m)/ (2\mathbf{a}_1.\mathbf{a}_2 \times \mathbf{a}_3) : 1,m,n = 1,2,3$

where ϵ_{klm} is the Levi-Civita tensor with the properties
ϵ_{klm} = +1 if l,m,n = 1,2, 3 respectively or any cyclic permutation
= 0 if any index is repeated
= -1 otherwise

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Any reciprocal lattice vector may, therefore, be written as

(3a,b) $\mathbf{g} = g_k \mathbf{b}_k = (2\pi) n_k \mathbf{b}_k$; k = 1,2,3

where n_1, n_2, n_3 are integers. This condition is obtained by applying the periodicity condition $f(\mathbf{r} + \mathbf{L}) = f(\mathbf{r})$ on the Fourier transform of f(r). The reciprocal lattice vectors satisfy the conditions

$$\mathbf{a}_i.\mathbf{b}_j = \delta_{ij}$$

where

$$\delta_{ij} = 1 \text{ if } i = j$$
$$= 0 \text{ otherwise}$$

A Dimensionless Lattice

Since the reciprocal lattice vectors have dimensions of $(\text{length})^{-1}$, they will be associated with a particular system of units. We need to construct a set of lattice vectors which is independent of the coordinate system used. Let us take the cross product of the direct lattice vectors and the reciprocal lattice vectors. The resulting vectors c_1, c_2 c_3 termed as cross lattice vectors are given by (Kamal and Hussain, 1978)

(5a,b,c) $\mathbf{c}_1 = \mathbf{a}_1 \times \mathbf{b}_1$, $\mathbf{c}_2 = \mathbf{a}_2 \times \mathbf{b}_2$, $\mathbf{c}_3 = \mathbf{a}_3 \times \mathbf{b}_3$

The *cross lattice length* can be written as

(6a,b) $\mathbf{D} = D_k \mathbf{c}_k = (2\pi) n_k \mathbf{c}_k$; k = 1,2,3

Since $\mathbf{L} = L_k \mathbf{a}_k$, $\mathbf{g} = g_k \mathbf{b}_k$ we note that

(7a,b) $\mathbf{D}.\mathbf{L} = 0$, $\mathbf{D}.\mathbf{g} = 0$

and so

(8a,b) $\exp(i\mathbf{D}.\mathbf{L}) = 1$, $\exp(i\mathbf{D}.\mathbf{g}) = 1$

whatever may be the values of L and g.

Eigenfunctions

In analogy with the momentum eigenfunctions and Wannier functions (Wannier, 1937; Kohn, 1973), it is desirable to obtain the eigenfunctions of cross lattice also. Supposing that the potential does not depend on the radial distance but it depends on the direction i.e. the potential can be expressed in terms of angle θ. If θ is a vector from the reference point to the point under consideration and proportional in magnitude to the angle θ, the potential can be expressed as a function of s. Expanding the Fourier series we get

$$(9) \qquad V(s) = \sum_{D_n} V(D_n) \exp(iD_n.s)$$

where $V(D_n)$ is a Fourier coefficient associated with a point in cross lattice and is given by

$$(10) \qquad V(D_n) = U^{-1} \int_{unit\ cell} V(s) \exp(-1D_n.s)$$

where U is the volume of the unit cell. The other periodic function is a Bloch-type function.

$$(11) \qquad u_D(s) = \sum_{D_n} v_D(D_n) \exp(iD_n.s) d\,s$$

where

$$(12) \qquad v_D(D_n) = K^{-1} \int_{unit\ cell} u_D(s) \exp(iD_n.s)\, ds$$

where k is the propagation number. For each value of D and each band there is a set of numbers $v_D(D_n)$ one for vector of the cross lattice and a convenient form of denoting them is $v(D - D_n)$. Therefore by multiplying (11) by exp(iD.S) we have the wavefunction

$$(13) \qquad \psi_D(s) = \sum v(D - D_n) \exp[i(D + D_n).S]$$

Since the wavefunctions $\exp[i(D + D_n).s]$ form an orthogonal set in unit cell, eq. (13) may be inverted to give

$$(14) \qquad v(D - D_n) = U^{-1} \int_{unit\ cell} \psi_D(s) \exp[-\iota (D + D_n).s] ds$$

The wavefunction ψ is normalized in the unit cell.

$$1 = \int_{unit\ cell} \psi_D^*(s)\psi_D(s) ds$$

$$= \sum_{D_m, D_n} v^*(D - D_n)\, v(D - D_m) \int_{unit\ cell} \exp[i(D_m - D_n).s] ds$$

$$= U \sum_{\mathbf{D}_m,\mathbf{D}_n} v^*(\mathbf{D} - \mathbf{D}_n)\, v(\mathbf{D} - \mathbf{D}_m)\ \delta(\mathbf{D}_m - \mathbf{D}_n)$$

Therefore the orthonormalization condition when ψ is normalized in the unit cell is given by

$$(15) \qquad \sum_{\mathbf{D}_m,\mathbf{D}_n} v^*(\mathbf{D} - \mathbf{D}_n)\, v(\mathbf{D} - \mathbf{D}_m) = U^{-1}\ \delta(\mathbf{D}_m - \mathbf{D}_n)$$

There is a similar condition for the eigenfunctions belonging to different bands k, l

$$(16) \qquad \sum_{\mathbf{D}_n} V_k^*(\mathbf{D} - \mathbf{D}_n)\, v_l(\mathbf{D} - \mathbf{D}_n) = U^{-1}\ \delta_{kl}$$

Therefore the square of the modulus of the cross eigenfunction multiplied by U gives the probability that the electron in the state D has angular momentum $(h/2\pi)$ $(\mathbf{D} - \mathbf{D}_n)$.

Discussion

The band must be well separated so that there are nondiagonal matrix elements with respect to the band index. Let us define a modified Brillouin zone to be a Wigner-Sietz cell in cross lattice. If we let D take all values inside a modified Brillouin zone all the coefficients vary and are functions of D, But because of the periodicity in the momentum space, they all are in fact the same functions of D, only displaced one with respect to other by vectors of the cross lattice.

Conclusion

The momentum eigenfunctions of the reciprocal lattice and the Wannier functions are useful for systems which are isotropic but *inhomogeneous*, the *cross eigenfunctions* (belonging to eigenstate of angalar momentum in cross lattice representation are useful for systems which are homogeneous but anisotropic. Future work in this direction may involve construction of eigenfunctions which are both *inhomogeneous* and anisotropic.

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