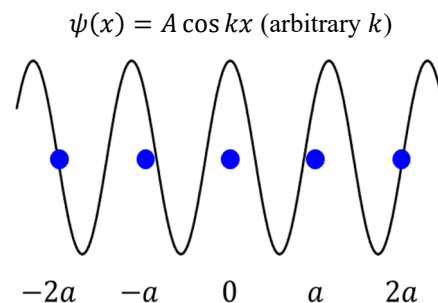


RECIPROCAL SPACE

(40) Periodic Functions on a Lattice: If $\psi(x)$ has the total symmetry of a 1-d Bravais lattice with distance a between adjacent lattice points, then

$$\psi(x + ma) = \psi(x)$$

for all integers m ? Naturally periodic functions include transcendental functions like $A \sin kx$ and $A \cos kx$ in which the *wavevector* k is related to the wavelength λ by $k = 2\pi/\lambda$. As a specific example, for any general value of k , the function $A \cos kx$ is *not periodic* with respect to this lattice, as seen to the right. However, for certain values of $k = K_h$, $A \cos K_h x$ is periodic with the lattice. The allowed values of K_h are determined by equating $\psi(x + a)$ with $\psi(x)$ because a represents the smallest repeating distance of the lattice:



$$A \cos K_h(x + a) = A \cos K_h x = A \cos K_h x \cos K_h a - A \sin K_h x \sin K_h a.$$

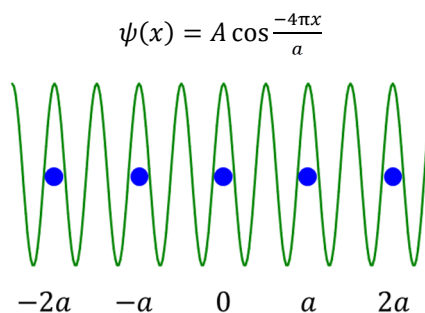
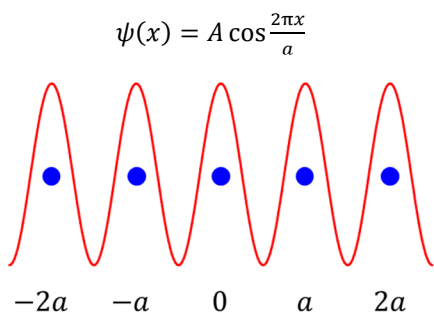
Since $\cos kx$ and $\sin kx$ are, respectively, even and odd functions with respect to inversion through the origin, the term $A \sin K_h x \sin K_h a$ must be eliminated, which means

$$\sin K_h a = 0, \text{ or } K_h a = 2\pi h \text{ for } h = \text{any integer.}$$

As a result, the values of K_h for which $A \cos K_h x$ is periodic on the 1-d lattice with spacing a between adjacent lattice points are

$$K_h = \dots, \frac{-6\pi}{a}, \frac{-4\pi}{a}, \frac{-2\pi}{a}, 0, \frac{2\pi}{a}, \frac{4\pi}{a}, \frac{6\pi}{a}, \dots,$$

as the following graphs illustrate for $K_h = \frac{2\pi}{a}$ and $\frac{-4\pi}{a}$:

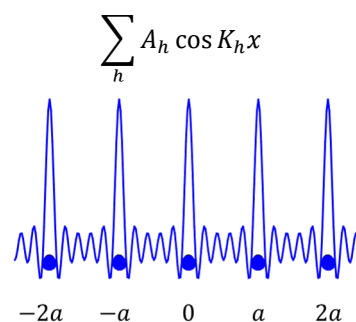


Both functions are, indeed, periodic on the lattice, but only the function $A \cos(2\pi x/a)$ repeats exactly by the lattice constant a . Among the other solutions, the resulting “wave” for $K_h = 0$ is a constant $\psi(x) = A$, while the others repeat by integer fractions of a , i.e., a/h . Furthermore, the restriction for the allowed values of K_h also applies to $A \sin K_h x$ and the complex plane wave $A e^{iK_h x} = A(\cos K_h x + i \sin K_h x)$.

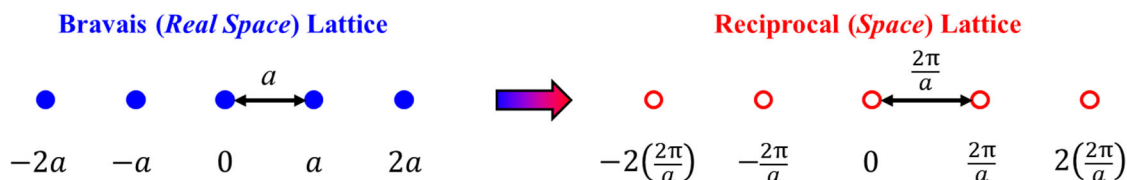
The most general periodic functions with respect to a 1-d lattice are *Fourier series*, i.e., sums of cosine and sine functions over all integers h :

$$\sum_h A_h \cos K_h x + B_h \sin K_h x \text{ or } \sum_h C_h e^{iK_h x}.$$

The infinite sums are truncated, which introduces oscillations in the final function, as shown to the right.



(41) The Reciprocal Lattice: The analysis of periodic functions on a 1-d Bravais lattice in *real space*, which is the set of points $\{\dots, -2a, -a, 0, a, 2a, \dots\}$, identifies a lattice in *reciprocal space*, which is the corresponding set of points $\{\dots, -4\pi/a, -2\pi/a, 0, 2\pi/a, 4\pi/a, \dots\}$.



The *reciprocal lattice* is the set of all wavevectors, with units $(\text{length})^{-1}$, that yield plane waves with the periodicity of the Bravais lattice.

For 3-d space, plane wave functions $\psi(\mathbf{r})$ that have the total symmetry of the 3-d Bravais lattice must obey the following equation:

$$\psi(\mathbf{r} + \mathbf{T}_{mnp}) = \psi(\mathbf{r}) = Ae^{i\mathbf{K}_{hkl}\cdot\mathbf{r}} = Ae^{i\mathbf{K}_{hkl}\cdot(\mathbf{r} + \mathbf{T}_{mnp})} = Ae^{i\mathbf{K}_{hkl}\cdot\mathbf{r}} Ae^{i\mathbf{K}_{hkl}\cdot\mathbf{T}_{mnp}},$$

which gives the conditions for the reciprocal lattice \mathbf{K}_{hkl} :

$$e^{i\mathbf{K}_{hkl}\cdot\mathbf{T}_{mnp}} = 1, \text{ or } \mathbf{K}_{hkl} \cdot \mathbf{T}_{mnp} = 2\pi \times \text{integer}.$$

To ensure that all reciprocal lattice points are identified, Bravais lattice vectors must be expressed using the primitive cell, i.e., $\mathbf{T}_{mnp} = m\mathbf{a}_1 + n\mathbf{a}_2 + p\mathbf{a}_3$; $m, n, p =$ all integers. Then, the conditions on \mathbf{K}_{hkl} become

$$\mathbf{K}_{hkl} \cdot \mathbf{a}_1 = 2\pi h; \quad \mathbf{K}_{hkl} \cdot \mathbf{a}_2 = 2\pi k; \quad \mathbf{K}_{hkl} \cdot \mathbf{a}_3 = 2\pi l; \quad h, k, l = \text{all integers}.$$

If every reciprocal lattice vector is expressed using its own primitive cell, i.e., $\mathbf{K}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$; $h, k, l =$ all integers, then the conditions defining the reciprocal lattice become

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij}; \quad (i, j = 1, 2, 3).$$

As a result, the primitive unit cell of the Bravais lattice in real space defines the primitive unit cell of the corresponding reciprocal lattice. The 1-d Bravais lattice is $\{\mathbf{T}_m = m\mathbf{a}\}$, the corresponding reciprocal lattice is $\{\mathbf{K}_h = h\mathbf{a}^*\}$, and the length of \mathbf{a}^* is $2\pi/a$.

(42) To summarize the results above, once a primitive unit cell in real space is identified, then the corresponding primitive cell of the reciprocal lattice can be calculated:

$$\text{Bravais Lattice: } \{\mathbf{T}_{mnp} = m\mathbf{a}_1 + n\mathbf{a}_2 + p\mathbf{a}_3; (m, n, p \text{ integers})\}$$

$$\text{Reciprocal Lattice: } \{\mathbf{K}_{hk} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*; (h, k, l \text{ integers and } \mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij})\}.$$

The conditions relating real space and reciprocal space primitive cell vectors means that \mathbf{a}_1^* is perpendicular to \mathbf{a}_2 and \mathbf{a}_3 , \mathbf{a}_2^* is perpendicular to \mathbf{a}_1 and \mathbf{a}_3 , and \mathbf{a}_3^* is perpendicular to \mathbf{a}_1 and \mathbf{a}_2 . According to these relationships, the primitive vectors of the reciprocal lattice can be determined from the primitive vectors of the real-space Bravais lattice as follows:

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}; \quad \mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}; \quad \mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}.$$

The numerators in each equation yield vectors that are orthogonal to the plane of the two vectors; the denominators are all the same and equal the volume of the primitive unit cell V_1 . Therefore,

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_1}; \quad \mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_1}; \quad \mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_1}.$$

VECTOR PRODUCTS: The expressions defining the primitive cell vectors of the reciprocal lattice use three important vector products, which are described below. In the following, vectors are denoted using boldface. $\mathbf{a} = a_x\hat{x} + a_y\hat{y} + a_z\hat{z}$ (length a), $\mathbf{b} = b_x\hat{x} + b_y\hat{y} + b_z\hat{z}$ (length b), and $\mathbf{c} = c_x\hat{x} + c_y\hat{y} + c_z\hat{z}$ (length c). Vectors with the carrot overhead, such as \hat{x} , have unit length.

Vector Dot (Scalar) Product of \mathbf{a} and \mathbf{b} :

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z = ab \cos \gamma; \gamma = \text{angle between } \mathbf{a} \text{ and } \mathbf{b}.$$

Vector Cross Product of \mathbf{a} and \mathbf{b} :

$$\mathbf{a} \times \mathbf{b} = \det \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{pmatrix} = (a_y b_z - a_z b_y)\hat{x} + (a_z b_x - a_x b_z)\hat{y} + (a_x b_y - a_y b_x)\hat{z}.$$

The length of $\mathbf{a} \times \mathbf{b}$ is $ab \sin \gamma$, $\gamma = \text{angle between } \mathbf{a} \text{ and } \mathbf{b}$; the orientation of $\mathbf{a} \times \mathbf{b}$ is perpendicular to the plane of \mathbf{a} and \mathbf{b} and directed according to the right-hand rule (using your right hand, if the direction of your index finger is the first vector \mathbf{a} and your other fingers curl toward the direction of the second vector \mathbf{b} , then the direction of your outstretched thumb is the direction of $\mathbf{a} \times \mathbf{b}$). The length of $\mathbf{a} \times \mathbf{b}$ is the area of the parallelogram formed by \mathbf{a} and \mathbf{b} .

Vector Triple Product of \mathbf{a} , \mathbf{b} , and \mathbf{c} :

$$\mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = \det \begin{pmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{pmatrix} = a_x(b_y c_z - b_z c_y) + a_y(b_z c_x - b_x c_z) + a_z(b_x c_y - b_y c_x).$$

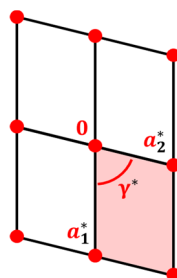
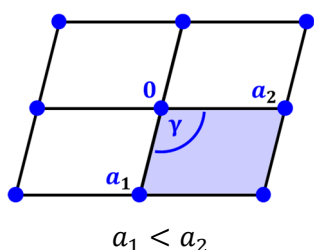
This scalar quantity is the volume of the parallelepiped formed by vectors \mathbf{a} , \mathbf{b} , and \mathbf{c} .

Using these formulas for determining primitive cell vectors for a reciprocal lattice, below are illustrated the reciprocal lattices for each of the five 2-d lattices (to accomplish the vector cross-product, choose \mathbf{a}_3 to be a unit vector oriented perpendicular to the 2-d Bravais lattice).

BRAVAIS LATTICE

RECIPROCAL LATTICE

OBLIQUE: $a_1 \neq a_2; \gamma \neq 90^\circ$

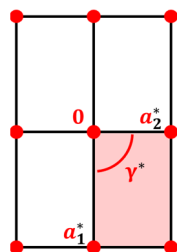
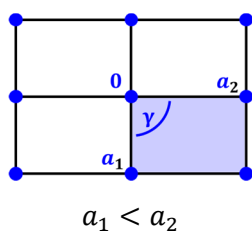


$$a_1^* = \frac{2\pi}{a_1 \sin \gamma}$$

$$a_2^* = \frac{2\pi}{a_2 \sin \gamma}$$

$$\gamma^* = 180^\circ - \gamma$$

RECTANGULAR: $a_1 \neq a_2; \gamma = 90^\circ$



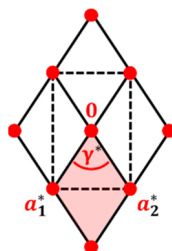
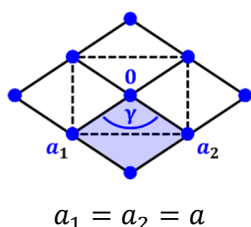
$$a_1^* = \frac{2\pi}{a_1}$$

$$a_2^* = \frac{2\pi}{a_2}$$

$$\gamma^* = 90^\circ$$

 CENTERED RECTANGULAR:

$$a_1 = a_2; \gamma \neq 90^\circ$$



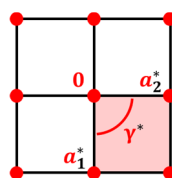
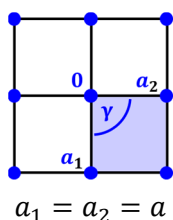
$$a_1^* = \frac{2\pi}{a \sin \gamma}$$

$$a_2^* = \frac{2\pi}{a \sin \gamma}$$

$$\gamma^* = 180^\circ - \gamma$$

TETRAGONAL:

$$a_1 = a_2; \gamma = 90^\circ$$



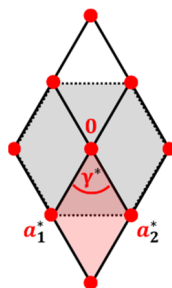
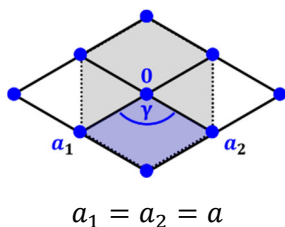
$$a_1^* = \frac{2\pi}{a}$$

$$a_2^* = \frac{2\pi}{a}$$

$$\gamma^* = 90^\circ$$

TRIGONAL/HEXAGONAL:

$$a_1 = a_2; \gamma = 120^\circ$$



$$a_1^* = \frac{2\pi}{a \sin 120^\circ} = \frac{4\pi}{\sqrt{3}a}$$

$$a_2^* = \frac{2\pi}{a \sin 120^\circ} = \frac{4\pi}{\sqrt{3}a}$$

$$\gamma^* = 60^\circ$$

Some conclusions inferred from these illustrations include:

- The rotational symmetry of the reciprocal lattice matches the rotational symmetry of the Bravais lattice. This is particularly emphasized by the gray-shaded hexagonal regions for the trigonal/hexagonal real space and reciprocal space lattices.
- The relative lengths of the primitive cell parameters of the reciprocal lattice are inversely related to the primitive cell parameters of the real space Bravais lattice.
- The reciprocal lattice for the centered rectangular Bravais lattice is also centered rectangular, but it must be calculated from the primitive unit cell.

In 3-d, the following relationships between real space Bravais lattices and reciprocal lattices hold:

- Primitive real space lattices give primitive reciprocal lattices;
- Base-centered (*C*- or *A*-) real space lattices give base-centered reciprocal lattices;
- Body-centered (*I*-) real space lattices give face-centered (*F*-) reciprocal lattices; and
- Face-centered (*F*-) real space lattices give body-centered (*I*-) reciprocal lattices.

The reciprocal lattice for a crystalline solid can be “observed” by diffraction experiments because the condition for constructive interference of diffracted radiation puts the observed diffracted waves at the positions of the reciprocal lattice. Each observable diffraction peak is labeled by its *Miller indices* (*hkl*).

PRACTICE EXERCISE: Determine the reciprocal lattice for a body-centered cubic real space Bravais lattice with cubic unit cell length a .

The body-centered cubic cell is $\mathbf{a} = a\hat{x}$; $\mathbf{b} = a\hat{y}$; $\mathbf{c} = a\hat{z}$. With lattice points at the corners and center of this cell, the primitive unit cell is

$$\mathbf{a}_1 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}; \quad \mathbf{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z}; \quad \mathbf{a}_3 = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}.$$

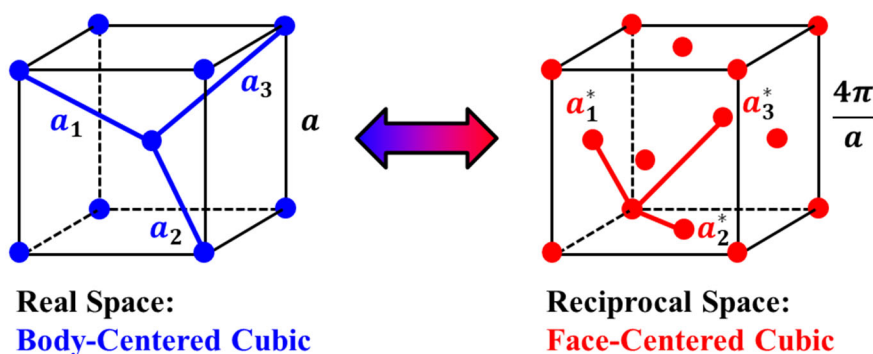
The volume of the primitive cell is $V_1 = a^3/2$. Then, using the formulas for the primitive cell vectors of the reciprocal lattice, we obtain

$$\mathbf{a}_1^* = \frac{4\pi}{a^3} \left[\frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \right] \times \left[\frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \right] = \frac{\pi}{a} [2(\hat{y} \times \hat{z}) + 2(\hat{x} \times \hat{y})] = \frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{z};$$

$$\mathbf{a}_2^* = \frac{4\pi}{a^3} \left[\frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \right] \times \left[\frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \right] = \frac{\pi}{a} [2(\hat{y} \times \hat{z}) + 2(\hat{z} \times \hat{x})] = \frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{y};$$

$$\mathbf{a}_3^* = \frac{4\pi}{a^3} \left[\frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \right] \times \left[\frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \right] = \frac{\pi}{a} [2(\hat{z} \times \hat{x}) + 2(\hat{x} \times \hat{y})] = \frac{2\pi}{a}\hat{y} + \frac{2\pi}{a}\hat{z}.$$

These vectors form the primitive cell for a face-centered cubic lattice. The side of the cubic cell is $4\pi/a$.



The reciprocal lattice partitions reciprocal space into cells and identifies those wavevectors that create plane waves that are periodic with the real space Bravais lattice. Now, what significance do the wavevectors in the region between reciprocal lattice points have?

(43) Irreducible Representations of the 1-d Translation Group: The group of translations in one-dimension is a quasi-infinite set of lattice translations $\mathcal{L} = \{(1|T_m), m = \text{integer}\}$. To make the problem tractable, periodic boundary conditions are applied to this set so that for any vector \mathbf{x} , $\mathbf{x} + T_N = \mathbf{x}$, i.e., T_N is equivalent to the identity translation $T_N = \mathbf{0}$. Since this group of translations is Abelian, each member is its own class and the number of irreducible representations (IRs) equals the number of members of the group. Therefore, each IR is one-dimensional.

As a concrete example, consider a 1-d lattice with lattice constant a and set the periodic boundary condition to be four primitive translations, i.e., $T_4 = \mathbf{0}$. Let $T_m \equiv (1|ma)$. Then, the set of translation operations that set the Bravais lattice contains 4 members:

$$\mathcal{L} = \{T_1, T_2, T_3, T_4 = T_0\} \equiv \{(1|a), (1|2a), (1|3a), (1|4a) = (1|0)\}.$$

Therefore, the group has 4 classes and, as a result, 4 1-dimensional IRs, which we can label as $\Gamma^{(1)}$, $\Gamma^{(2)}$, $\Gamma^{(3)}$, and $\Gamma^{(4)}$. Therefore, for each class of symmetry operations, the matrix representatives, which are also the characters of these IRs, must be complex numbers.

We use the properties of the group \mathcal{L} to determine the expressions for these characters. Start by determining the characters of each IR for the fundamental translation $T_1 \equiv (1|a)$. Let $\Gamma^{(\mu)}(T_1) = \varepsilon_\mu$. If the operation T_1 is performed 4 successive times, i.e.,

$$T_1^4 = (1|a)^4 = (1|4a) \equiv (1|0) = T_0, \text{ the identity,}$$

then $\epsilon_\mu^4 = 1$, which has the solutions $\epsilon_\mu = e^{-2\pi i \mu/4}$ for $\mu = 1, 2, 3, 4$:

$$\epsilon_1 = e^{-2\pi i(1)/4} = e^{-i\pi/2} = -i; \quad \epsilon_2 = e^{-2\pi i(2)/4} = e^{-i\pi} = -1;$$

$$\epsilon_3 = e^{-2\pi i(3)/4} = e^{-3i\pi/2} = +i; \quad \epsilon_4 = e^{-2\pi i(4)/4} = e^{-2i\pi} = +1.$$

We can use these characters to determine the characters for $\Gamma^{(\mu)}(T_m)$:

$$\Gamma^{(\mu)}(T_m) = \Gamma^{(\mu)}(mT_1) = [\Gamma^{(\mu)}(T_1)]^m = \epsilon_\mu^m = e^{-2\pi i m \mu/4}.$$

Therefore, the character or representative of $\Gamma^{(\mu)}(T_m)$ contains a label for the class (m) and for the IR (μ). Although this is a convenient formula, it is helpful and useful to relate this expression directly to the lattice vectors T_m rather than just the index m of the lattice vector. To accomplish this, we rewrite the exponent and do a fair amount of rearrangement:

$$\frac{2\pi i m \mu}{4} \cdot \frac{a}{a} = i \left(\frac{2\pi \mu}{4a} \right) (ma) = i \left[\frac{\mu}{4} \left(\frac{2\pi}{a} \right) \right] (ma) = i \mathbf{k}_\mu \cdot T_m.$$

In this rearrangement of the exponent, \mathbf{k}_μ is the *wavevector* or *k-point* associated with the IR $\Gamma^{(\mu)}$ of the Bravais lattice group \mathcal{L} . Therefore, the character or representative of the IR $\Gamma^{(\mu)}(T_m)$ for the lattice translation $T_m = (1|ma)$ is

$$\Gamma^{(\mu)}(T_m) = e^{-i \mathbf{k}_\mu \cdot T_m} = e^{-2\pi i m \mu/4}; \quad m, \mu = 1, 2, 3, 4,$$

in which m is a class label and μ is an IR label.

(44) This equation provides the means to construct the character table for this 1-d translation group. According to the periodic boundary condition $T_4 \equiv (1|4a) = (1|0) \equiv T_0$, there are 4 classes and, therefore, 4 irreducible representations, which are described by their wavevectors \mathbf{k}_μ :

| \mathcal{L} | T_0 | T_1 | T_2 | T_3 | Features of the Basis Functions | | |
|--|-------|-------|-------|-------|---------------------------------|-----------|--|
| | | | | | Real | Imaginary | |
| $k_1 = \frac{\pi}{2a} \quad \Gamma^{(1)}$ | 1 | -i | -1 | i | φ_1 | | |
| $k_2 = \frac{\pi}{a} \quad \Gamma^{(2)}$ | 1 | -1 | 1 | -1 | φ_2 | | |
| $k_3 = \frac{3\pi}{2a} \quad \Gamma^{(3)}$ | 1 | i | -1 | -i | φ_3 | | |
| $k_4 = \frac{2\pi}{a} \quad \Gamma^{(4)}$ | 1 | 1 | 1 | 1 | φ_4 | | |

The basis functions $\varphi_\mu(x)$ must satisfy the following equation:

$$(1 | ma) \varphi_\mu(x) = e^{-i \mathbf{k}_\mu \cdot ma} \varphi_\mu(x),$$

which describes how the symmetry operations (lattice translations) affect the basis function for the IR $\Gamma^{(\mu)}$. To illustrate this important feature of basis functions, a real function (yellow half-ellipse with solid red boundary) is placed at the origin lattice point 0. For each IR, the effect of the translation is illustrated: a change of sign flips the half-ellipse with respect to the real line and a change to an imaginary value gives a green half-ellipse with dashed blue boundary.

OBSERVATIONS:

- (a) The characters for the class T_0 are all unity, in agreement with the assignment that this translation corresponds to the identity operation of the group.
- (b) Each basis function obeys the periodic boundary condition: $\varphi_\mu(x + 4a) = \varphi_\mu(x)$.
- (c) The characters for the IR $\Gamma^{(4)}$ are all unity, so this IR is the *totally symmetric IR* of the lattice group and its basis function $\varphi_4(x)$ has the complete symmetry of the Bravais lattice. The wavevector k_4 is $2\pi/a$, which is a reciprocal lattice vector, so the wavevector $k_0 = 0$ also yields the same characters. So, $k_0 = 0$ is chosen for the wavevector of this IR rather than $k_4 = 2\pi/a$.
- (d) The characters for the IR $\Gamma^{(2)}$ are the real numbers +1 or -1, so this IR is a *real representation* of the lattice group. Odd lattice steps change the sign of the basis function; even lattice steps retain the sign of the basis function.
- (e) The IRs $\Gamma^{(1)}$ and $\Gamma^{(3)}$ have imaginary characters and they occur as complex conjugate pairs. Therefore, their corresponding basis functions are complex conjugates of each other.

The four wavevectors of the four IRs, $k_0 = 0, k_1 = \pi/2a, k_2 = \pi/a, k_3 = 3\pi/2a$, represents points in reciprocal space between the two adjacent lattice points $k_0 = 0$ and $k_4 = 2\pi/a$. For this very restricted periodic boundary condition, the allowed wavevectors (“*k*-points”) form a discrete set that serve as labels for the IRs.

(45) The previous example illustrated how the IRs arise for a set of lattice translations. In the example, the periodic boundary condition was set low, but they are generally selected to be quite large so that $T_{N_1} \equiv \mathbf{0}$ for a large integer N_1 . The resulting set of N_1 wavevectors k_μ form a set of very closely spaced, *quasi-continuous*, points in the *reciprocal space* of the periodic structure. The following summarizes this outcome for 1-d and 3-d Bravais lattices:

1-d Bravais Lattice $\mathcal{L} = \{(1|ma_1); 0 \leq m < N_1\}; N_1a_1 \equiv \mathbf{0}$.

Reciprocal lattice is $\{K_h = ha_1^*\}$ with $a_1^* = 2\pi/a$.

IR representatives are $\Gamma^{(\mu)} = e^{-ik_\mu ma}$ with wavevectors $k_\mu = \frac{\mu}{N_1} a_1^*$ ($0 \leq \mu < N_1$).

There are N_1 classes and N_1 IRs.

3-d Bravais Lattice $\mathcal{L} = \{(1|ma_1 + na_2 + pa_3); 0 \leq m < N_1, 0 \leq n < N_2, 0 \leq p < N_3\};$

$N_1a_1 \equiv \mathbf{0}, N_2a_2 \equiv \mathbf{0},$ and $N_3a_3 \equiv \mathbf{0}$.

Reciprocal lattice is $\{K_{hkl} = ha_1^* + ka_2^* + la_3^*\}$.

IR representatives are $\Gamma^{(\mu\nu\omega)} = e^{-ik_{\mu\nu\omega} \cdot T_{mnp}} = \exp\left(-2\pi i \left(\frac{\mu m}{N_1} + \frac{\nu n}{N_2} + \frac{\omega p}{N_3}\right)\right)$ with

wavevectors $k_{\mu\nu\omega} = \frac{\mu}{N_1} a_1^* + \frac{\nu}{N_2} a_2^* + \frac{\omega}{N_3} a_3^*$ ($0 \leq \mu < N_1; 0 \leq \nu < N_2; 0 \leq \omega < N_3$).

There are $N_1N_2N_3$ classes and $N_1N_2N_3$ IRs.

Now that we have identified the irreducible representations for the group of lattice translations, *what are the basis functions for these IRs?* As we pointed out in slide **(38)**, these functions serve as eigenfunctions for the one-electron Schrödinger equation. For the 1-d example, we illustrated important features of these basis functions based upon how they are affected by the various translational symmetry operations of the lattice.