Lattice symmetry and Bloch's Theorem

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Outline

Symmetry
- Symmetry Operations
- Eigenstates and Irreducibility

Lattices
- Bravais Lattice
- Reciprocal Lattice
- Space Group

Bloch's Theorem
- Proof
- Examples

Symmetry Operations

- Consider a symmetry operation R that transforms coordinates $\boldsymbol{r}$ to $\boldsymbol{r}'$ as

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- Upon dropping the primes, we reach the definition of the operator P_R on the function space

$$\boxed{P_R\psi(\boldsymbol{r}) = \psi(R^{-1}\boldsymbol{r})} \tag{2}$$

Symmetry Operations

- Restricting $\psi(\boldsymbol{r})$ to be a wavefunction of a quantum mechanical system requires P_R to be a unitary operator to preserve the inner product between two functions

$$\langle \phi(\boldsymbol{r}), \psi(\boldsymbol{r}) \rangle = \int \phi^*(\boldsymbol{r}) \psi(\boldsymbol{r}) d^3\boldsymbol{r}, \tag{3}$$

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- Let T be a quantum mechanical operator that transforms to T' upon the operation R. The requirement

$$\langle \phi, T\psi \rangle = \langle P_R\phi, T'P_R\psi \rangle \implies \langle P_R\phi, P_RT\psi \rangle = \langle P_R\phi, T'P_R\psi \rangle$$

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- The above equality holds for arbitrary functions only when

$$T' = P_RTP_R^{-1} \implies T - T' = [T, P_R]P_R^{-1}, \tag{4}$$

  which defines the transformation law for operators. It also show that T is invariant under P_R iff $[T, P_R] = 0$.

Hamiltonian Symmetry

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- A Hamiltonian is invariant under a symmetry operation R if

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  or equivalently $[H, R] = 0$.
- Consider the set G of all symmetry operations $\{R_1, R_2, \dots\}$ with the binary operation $R_i R_j$. G satisfies:
  - Closure: $(R_i R_j) H (R_i R_j)^{-1} = H \implies R_i R_j \in G$
  - Associativity: since they are quantum mechanical operators.
  - Identity: because $\varepsilon H \varepsilon^{-1} = H$.
  - Unique inverse: since $RHR^{-1} = H \implies H = R^{-1} H R \implies R^{-1} \in G$

  Then G is a group.

Eigenstates and Representation

- Now consider a Hamiltonian H that has a d-fold degenerate subspace V with energy level E. This subspace can be spanned by basis ϕ_n, which are also eigenstates of H

$$H\phi_n = E\phi_n, \quad n = 1, 2, \ldots, d \tag{5}$$

where $\langle \phi_n, \phi_m \rangle = \delta_{nm}$.

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- A symmetry operation $R \in G$ commutes with H so Eq. (5) transforms to

$$H(R\phi_n) = E(R\phi_n) \implies R\phi_n \in V \implies R\phi_n = \sum_{m=1}^{d} \phi_m D_{mn}(R)$$

  where $D_{mn}(R) = \langle \phi_m, R\phi_n \rangle$ are the elements of a matrix $D(R)$.

Eigenstates and Representation

- The matrices $D(R)$ form a representation of the group G.

$$D(R_1R_2)_{mn} = \langle \phi_m, R_1R_2\phi_n \rangle = \sum_k D_{kn}(R_2)\langle \phi_m, R_1\phi_k \rangle$$
$$= \sum_k D_{kn}(R_2)D_{mk}(R_1) = \Big(D(R_1)D(R_2)\Big)_{mn}$$

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- The representation D is irreducible [1].
- Example: Degenerate sub-spaces of a spherically symmetric Hamiltonian have eigenstates given by spherical Harmonics $Y_{lm}(\theta, \phi)$. These are the basis for irreps D^l with $\dim D^l = 2l + 1$.

Lattice

- A Lattice (Bravais Lattice) is a space-filling array of points generated by three primitive lattice vectors $\boldsymbol{t}_1, \boldsymbol{t}_2$, and $\boldsymbol{t}_3$. A general point in the lattice could be represented by a vector

$$\boldsymbol{t}_n = n_1\boldsymbol{t}_1 + n_2\boldsymbol{t}_2 + n_3\boldsymbol{t}_3 \tag{6}$$

  where $n = (n_1, n_2, n_3)$ and $n_i \in \mathbb{Z}$. $\boldsymbol{t}_n$ are called *primitive translation vectors*.

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- In general, a lattice can have rotational symmetry. However, the compatibility of this symmetry with the translation symmetry in Eq. (6) imposes restrictions on the rotational symmetry of a lattice.

Possible Bravais Lattices

- An arbitrary primitive translation vector $\boldsymbol{t}_n$ rotated to $\alpha\boldsymbol{t}_n$ must also be a primitive lattice vector to satisfy the translation symmetry. This forces the rotation angle to be $2\pi/n$ for an integer n.

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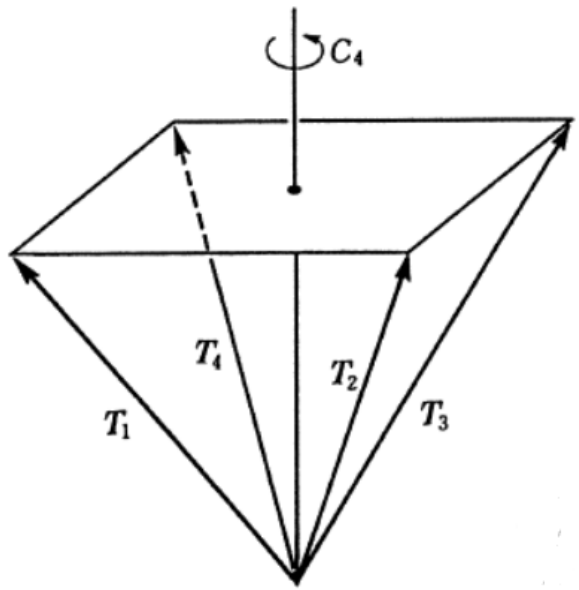
- An arbitrary primitive translation vector $\boldsymbol{t}_n$ rotated to $\alpha\boldsymbol{t}_n$ must also be a primitive lattice vector to satisfy the translation symmetry. This forces the rotation angle to be $2\pi/n$ for an integer n.
- If one considers a vector $\boldsymbol{T}_1$ and its successive rotations $\boldsymbol{T}_2, \ldots, \boldsymbol{T}_n$ shown in Fig. 9, we see that the vector $\sum_i \boldsymbol{T}_i$ is parallel to the axis of rotation C_n. Hence, any rotation axis is also a primitive translation vector.



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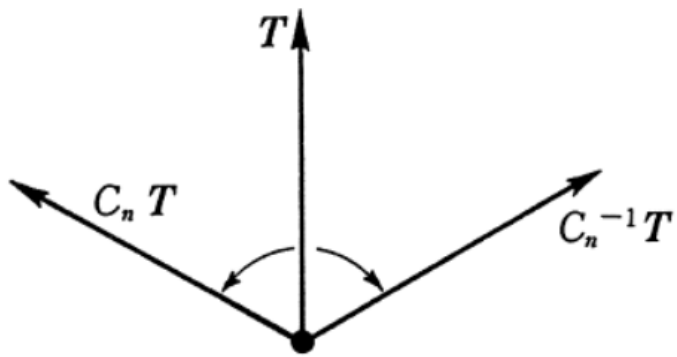
Possible Bravais Lattices

- In addition, all vectors $\boldsymbol{T}_i - \boldsymbol{T}_j$ are perpendicular to the axis of rotation.
- Pick the shortest vector $\boldsymbol{T}$ that is perpendicular to the axis of rotation of C_n. The rotation around that axis and it's inverse are shown in Fig. 2. It follows that

$$C_n\boldsymbol{T} + C_n^{-1}\boldsymbol{T} = 2\boldsymbol{T}\cos(2\pi/n) \implies \cos(2\pi/n) = \frac{\text{integer}}{2}$$

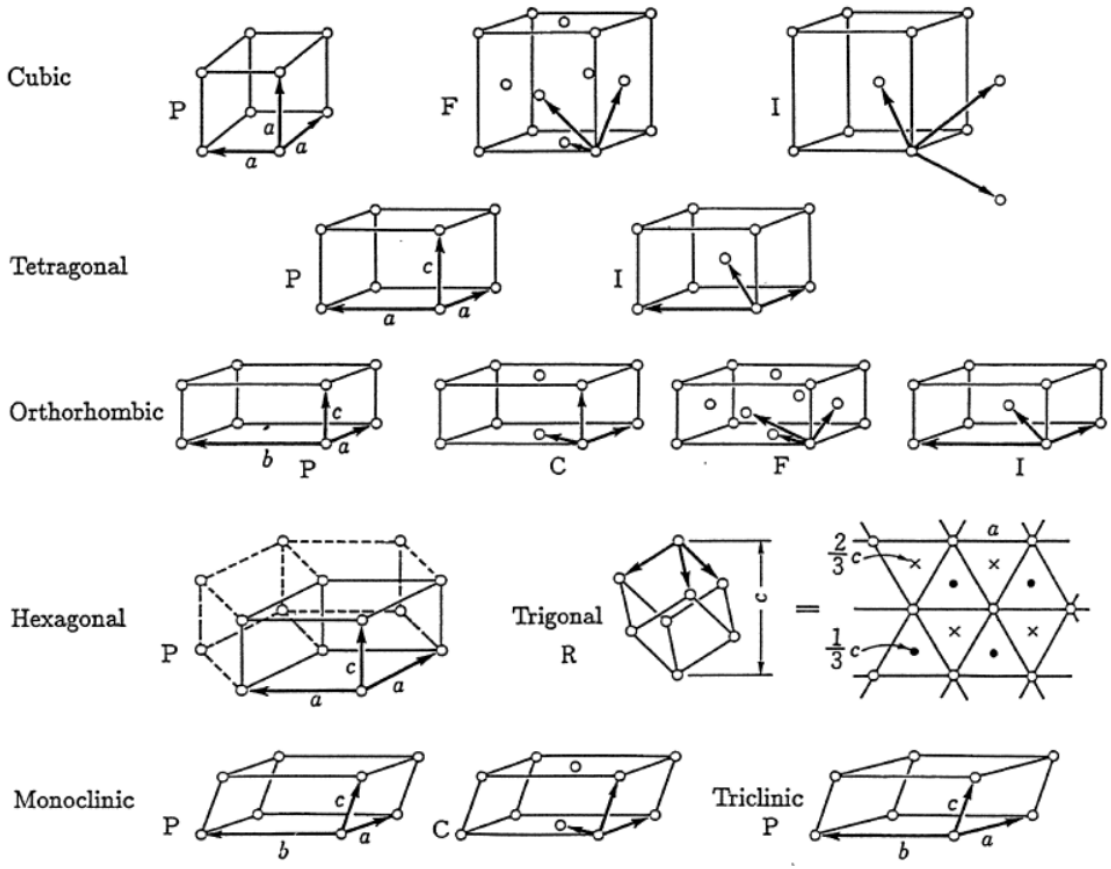
This restricts the rotation angles to be for $n = 1, 2, 3, 4, 6$.



[1]

Possible Bravais Lattices

The condition on *n* gives only 14 distinct lattices. These are shown in Fig. 3



[1]

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Reciprocal Lattice

- For a periodic function $f(\boldsymbol{r}) = f(\boldsymbol{r} - \boldsymbol{t}_n)$, the Fourier series expansion in terms of plane waves gives a condition on $\boldsymbol{k}$ due to the periodicity. Namely,

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \tilde{f}_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \implies e^{i\boldsymbol{k}\cdot\boldsymbol{t}_n} = 1$$

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- This shows that the space $\boldsymbol{k}$ is also periodic and the its basis $\{\boldsymbol{k}_i\}$ satisfy the condition $\boldsymbol{k}_i \cdot \boldsymbol{t}_j = 2\pi\delta_{ij}$. This condition is solved by

$$\boldsymbol{k}_a = \frac{2pi}{\Omega}(\boldsymbol{t}_b \times \boldsymbol{t}_c)$$

  where (a, b, c) are permutations of $(1, 2, 3)$, and $\Omega = \boldsymbol{t}_1 \cdot (\boldsymbol{t}_2 \times \boldsymbol{t}_3)$ is the volume of the unit cell in the spatial lattice. A general vector in this space is given by

$$\boldsymbol{k}_m = m_1\boldsymbol{k}_1 + m_2\boldsymbol{k}_2 + m_3\boldsymbol{k}_3$$

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- The unit cell of this lattice is called the *Brillouin zone*.

Space Group

- The point group and translation symmetry operations that keep the crystal invariant form a group called the *space group* [2]. A general element of a space group is written as

$$\{R|\boldsymbol{t}_n\}$$

where R is a point group element and $\boldsymbol{t}_n$ is the translation operations of the crystal. The action on coordinate $\boldsymbol{r}$ is

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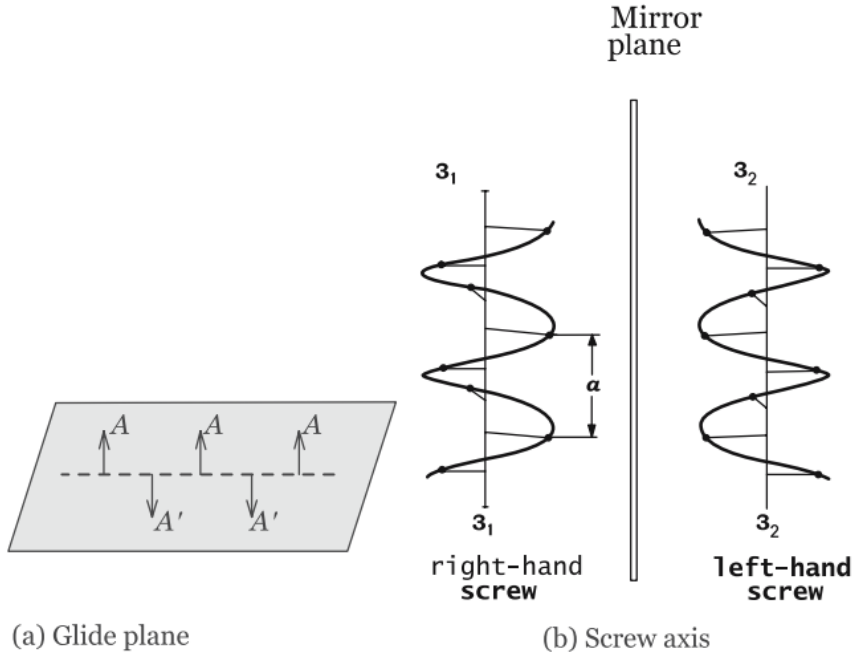
- The inverse of an element according to the multiplication law is

$$\{R|\boldsymbol{t}_n\}^{-1} = \{R^{-1}| - R^{-1}\boldsymbol{t}_n\}$$

Space Group

- Some operations in the space group are compound operations. There are 2 kinds of compound operations, which are shown in Fig. 4



[2]

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- There are 230 space groups generated by placing atoms on the distinct Bravais lattices.

Bloch's Theorem

For a Hamiltonian H that is invariant under translation by any primitive lattice vector, the eigenfunctions of the equation

$$H\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

are of the form

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$$

where n are different energy bands, $\boldsymbol{k}$ is a vector in the 1^{st} Brillouin zone, and $u_{n\boldsymbol{k}}(\boldsymbol{r})$ is a function with the same translation symmetry as H.

Proof of Bloch's Theorem

- A translation operation can be expressed as

$$\{\varepsilon|n_i\boldsymbol{t}_i\} = \{\varepsilon|n_1\boldsymbol{t}_1\}\{\varepsilon|n_2\boldsymbol{t}_2\}\{\varepsilon|n_3\boldsymbol{t}_3\}$$

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- If we impose periodic boundary conditions

$$\{\varepsilon|N_1\boldsymbol{t}_1\} = \{\varepsilon|N_2\boldsymbol{t}_2\} = \{\varepsilon|N_3\boldsymbol{t}_3\} = \{\varepsilon|0\}$$

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  where N_i is the number of lattice points along the direction of t_i. This allows us to study the bulk properties of the lattice and ignore the surface effects.
- Since T_i is an abelian group, all its irreducible representations are 1-dimensional. Therefore

$$D\left(\{\varepsilon|N_1\boldsymbol{t}_1\}\right) = D\left(\{\varepsilon|\boldsymbol{t}_1\}\right)^{N_1} = 1 \implies D_{p_1}\left(\{\varepsilon|\boldsymbol{t}_1\}\right) = e^{2\pi i p_1/N_1}$$

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- A triplet of integers (p_1, p_2, p_3) will determine an irrep of the group T, which the group of all the 3-dimensional translations of the lattice.
- Define the vector $\boldsymbol{k} = \frac{2\pi p_i \boldsymbol{k}_i}{N_i}$, and every irrep of T will be labeled by

$$D_{\boldsymbol{k}}\left(\{\varepsilon|\boldsymbol{t}_n\}\right) = e^{i\boldsymbol{k}\cdot\boldsymbol{t}_n}$$

  Replacing $\boldsymbol{k}$ by $\boldsymbol{k} + \boldsymbol{k}_m$ from the primitive translation vectors of the reciprocal lattice keeps the representation unaffected; hence, we can confine $\boldsymbol{k}$ to the first Brillouin zone.

Proof of Bloch's Theorem

- According to the transformation law in Eq. (2) on any function $\psi(\boldsymbol{r})$

$$\{\varepsilon|\boldsymbol{t}_n\}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} - \boldsymbol{t}_n)$$

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- Finally, plugging $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}((r))$ into the above equality, one gets the the condition that

$$u_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r} - \boldsymbol{t}_n) = \{\varepsilon|\boldsymbol{t}_n\}u_{\boldsymbol{k}}(\boldsymbol{r}),$$

  which complete the proof by shown that $u_k(\boldsymbol{r})$ has the same symmetry as the Hamiltonian.

A Chain of Finite Square Wells

Let

$$U(x) = \begin{cases} -V_0, & |x| \leq a \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

be the potential of a square well that is centered at the origin. Thus, the periodic potential we would like to solve can then be written as

$$V(x) = \sum_{s=-\infty}^{\infty} U(x - s(2a + b)) \tag{8}$$

Where b is the separation between the edges of the wells.

A Chain of Finite Square Wells

Such a periodic potential can be solved using Bloch's theorem, which gives the solutions as

$$\psi_{n,k}(x) = \sum_{r=-\infty}^{\infty} \phi_n(x - r(2a+b))e^{irk(2a+b)} \tag{9}$$

where $\phi_n(x)$ is the n^{th} eigenstate of the potential $U(x)$, and k is some crystal wave vector.
Schrodinger equation now reads

$$\hat{H}\psi_{n,k}(x) = E_{n,k}\psi_{n,k}(x) \tag{10}$$

where

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) = \frac{\hat{p}^2}{2m} + U(x) + \sum_{s\neq 0} U(x - s(2a+b))$$

A Chain of Finite Square Wells

Using Dirac (bracket) notation, and multiplying both sides by $\langle\phi_n|$

$$\langle\phi_n|\hat{H}|\psi_{n,k}\rangle = E_{n,k}\langle\phi_n|\psi_{n,k}\rangle$$

Notice that

$$\langle\phi_n|\frac{\hat{p}^2}{2m} + U(x)|\psi_{n,k}\rangle = E_n\langle\phi_n|\psi_{n,k}\rangle$$

Where E_n is the n^{th} eigenvalue of the potential $U(x)$, hence

$$E_{n,k} = E_n + \frac{\langle\phi_n|\sum_{s\neq 0} U(x - s(2a+b))|\psi_{n,k}\rangle}{\langle\phi_n|\psi_{n,k}\rangle}$$

A Chain of Finite Square Wells

Starting with the denominator, note that this is the probability of finding the particle in the central well, given that it's in the state $\psi(x)$. Each term of the summation calculates the probability of finding the particle in a specific well given that it's in the central well. This probability decreases drastically as the distance between the two wells increase. Thus, it suffices to include only the nearest neighbors of the central well.

$$\begin{aligned}\langle \phi_n | \psi_{n,k} \rangle &= \sum_{r=-\infty}^{\infty} e^{irk(2a+b)} \int_{-\infty}^{\infty} \phi_n(x - r(2a+b)) \phi_n^*(x) dx \\ &\approx 1 + 2\bar{\gamma_n} \cos\left(k(2a+b)\right)\end{aligned} \tag{11}$$

Where

$$\bar{\gamma_n} = \int_{-a}^{2a+b} \phi_n(x - (2a+b)) \phi_n^*(x) dx$$

A Chain of Finite Square Wells

And the numerator

$$\begin{aligned}\langle \dots \rangle &= \int_{-\infty}^{\infty} \phi_n^*(x) \Big(\sum_{s\neq 0} U(x - s(2a+b)) \Big) \Big(\sum_r \phi_n(x - r(2a+b)) e^{irk(2a+b)} \Big) dx \\ &\approx -2\gamma_n \cos\left(k(2a+b)\right)\end{aligned} \tag{12}$$

where

$$\gamma_n = V_0 \int_{a+b}^{3a+b} \phi_n(x - (2a+b)) \phi_n^*(x) dx$$

and we made use of the fact that $\phi_n(x) = \phi_n(-x)$. Therefore, the energy bands are then

$$E_{n,k} = E_n - \frac{2\gamma_n \cos\left(k(2a+b)\right)}{1 + 2\bar{\gamma}_n \cos\left(k(2a+b)\right)} \approx E_n - 2\gamma_n \cos\left(k(2a+b)\right) \tag{13}$$

because we expect $\bar{\gamma}_n \ll 1$.

Questions?

References

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Thank You!

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