Quantum Transport:

Atom to Transistor

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Lecture 13: Basis Functions as a Conceptual Tool

Ref. Chapter 4.2

Network for Computational Nanotechnology

nanoHUB
online simulations and more

Retouch on Concepts

00:00

- Recall, $EF = H_{op}F$ and

$$\Phi(\vec{r}) = \sum_m f_m u_m(\vec{r})$$

Where u_m are the basis functions.

- In matrix form,
$E[S]\{F\} = [H]\{F\}$ where the elements of [S] are

$$S_{mn} = \int d\vec{r} u_m^* u_n$$

and of [H]

$$H_{mn} = \int d\vec{r} u_m^* H_{op} u_n$$

- Main idea: Express a function as a linear combination of just a few functions and thus simplify computations. e.g. with Hydrogen we developed a 2x2 matrix from Φ_L and Φ_R.

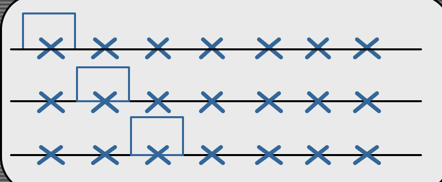
- Computationally, the most intensive part of this method lies in evaluating the elements of [S] and [H]

- Basis functions are also a very useful conceptual tool as we will discuss in this lecture

Finite Differences: “Pulse” Basis

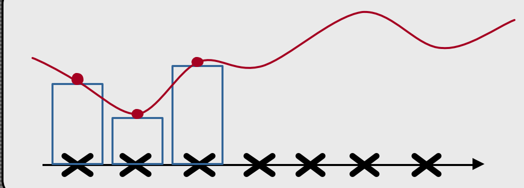
03:28

• In using the finite difference method, you can view basis set as the unit pulses centered around lattice points. This set can easily be seen to be orthogonal.



• With the coefficient factor f_m proportional to the height of $\Phi(\vec{r})$ at each lattice point .

$\Phi(\vec{r})$ Expanded as sum of Pulses



• Note: it is difficult to construct the Hamiltonian of this basis set because the first derivative of a pulse is two delta functions; hence the second derivative becomes even more complicated.

• A careful choice of basis functions, more complex than simple pulses, can improve accuracy and reduce computational time

Hilbert Space

06:59

- We know that a function may be expressed as a linear combination of basis functions:

$$\Phi(\vec{r}) = \sum_m f_m u_m(\vec{r})$$

- This is analogous to 3D space where any vector may be written as a linear combination of the Cartesian unit vectors:

$$\vec{V} = V_x \hat{x} + V_y \hat{y} + V_z \hat{z}$$

- Whereas for $\Phi(\vec{r})$ we have

$$\Phi(\vec{r}) = f_1 u_1 + f_2 u_2 + f_3 u_3 \cdots$$

- … Which, intuitively, can be thought of as a higher dimensional space for functions (often called a Hilbert Space).

- A concept fundamental to all vector spaces is the dot product. With 3D Cartesian vectors it is expressed as

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y + a_z b_z$$

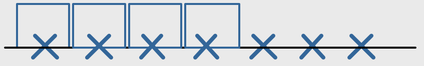
and in Hilbert Space it is

$$\int d\vec{r} f^*(\vec{r}) g(\vec{r})$$

Hilbert Space: Dot Product and Orthogonality

10:50

• In a discrete 1D lattice…



… the dot product is expressed as

$$\int dx f^*(x) g(x) = a \sum_m f^*(x_m) g(x_m)$$

where x_m are lattice points

• How do we define orthogonality using this definition of dot product?

• Two basis functions are orthogonal if

$$\int dx f^*(x) g(x) = 0$$

or in vector space $\vec{a} \cdot \vec{b} = 0$

• In choosing a coordinate system, orthogonal basis are usually chosen because they are easier to deal with. Sometimes it is advantageous to use oblique basis functions but that makes the problem conceptually harder.

• A commonly used expression for orthogonal basis functions is the "Kronecker Delta":

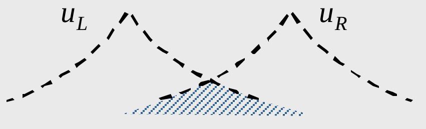
$$\int dx u_m^*(x) u_n(x) = d_{mn} = \begin{cases} 1, \text{if } m = n \\ 0, \text{if } m \neq n \end{cases}$$

Hilbert Space: Orthogonalizing a non-orthogonal basis

18:47

- Suppose we have a non-orthogonal set of basis functions.

e.g. H_2 from the last lecture:



- Such non-orthogonal basis functions may be transformed into a set of orthogonal basis functions. One way to do this is:

$$\tilde{u}_i(\vec{r}) = \sum \left[S^{-1/2}\right]_{ni} u_n(\vec{r})$$

Where $\tilde{u}_i(\vec{r})$ is the set of orthogonal functions

- The proof is as follows:

Let $\tilde{u}_j = \sum_m \left[S^{-1/2}\right]_{mj} u_m(\vec{r}),$ (1)

For orthogonality we should have:

$$\int d\vec{r}\, \tilde{u}_i^* \tilde{u}_j = 0 \quad (2)$$

Evaluating the left side of 2 using 1:

$$= \sum_n \left[S^{-1/2}\right]_{ni}^* \int d\vec{r} u_n^* \sum_m \left[S^{-1/2}\right]_{mj} u_m$$

$$= \sum_m \sum_n \left[S^{-1/2}\right]_{ni}^* S_{nm} \left[S^{-1/2}\right]_{mj}$$

where $\left(S_{nm} = \int d\vec{r} u_m^* u_n\right)$

Hilbert Space: Orthogonalizing a non-orthogonal basis

25:00

- So far we have:

$$\int d\bar{r}\,\tilde{u}_{i^*}\tilde{u}_j = \sum_m \sum_n \left[S^{-1/2}\right]^*_{ni} S_{mn} \left[S^{-1/2}\right]_{mj}$$

but the S matrix has the property

$$\left[S^{-1/2}\right]^*_{ni} = \left[S^{-1/2}\right]_{in}$$ therefore,

$$\int d\bar{r}\,\tilde{u}_{i^*}\tilde{u}_j = \sum_m \sum_n \left[S^{-1/2}\right]_{in} S_{mn} \left[S^{-1/2}\right]_{mj}$$

$$= [S^{-1/2}\, S\, S^{-1/2}]_{ij} = d_{ij}$$

- So $\tilde{u}_j$'s is in fact an orthogonal set and

$$\tilde{U}_i = \sum_n \left[S^{-1/2}\right]_{ni} U_n$$

is a transformation to an orthogonal set.

- Main Point: an orthogonal basis can always be constructed from a non-orthogonal basis

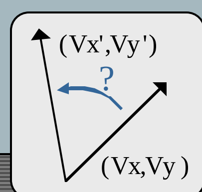
Operators: Rotation in Hilbert Space

Time – 28:35

• One might ask the question: "Why for a given operator the matrix elements are given as

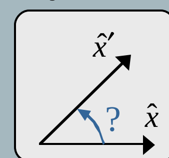
$$H_{nm} = \int d\bar{r}\, u_{n^*}(\bar{r}) H_{op} u_m(\bar{r}) \ ?"$$

• Essentially, this is because such operators act as linear transformers in Hilbert space. This occurs in much the same manner as it does in the conventional (x,y) Cartesian space. For example, consider an (x,y) rotation:



• How do we formulate this rotation? Well, begin by considering how it operates on the $\hat{x}$ and $\hat{y}$ unit basis vectors …

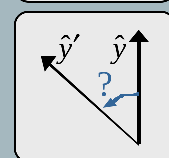
x :



$$\text{let } \hat{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\therefore\ \hat{x}' = \begin{bmatrix} \cos q & 0 \\ \sin q & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

y :



$$\text{let } \hat{y} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\therefore\ \hat{y}' = \begin{bmatrix} 0 & -\sin q \\ 0 & \cos q \end{bmatrix}$$

Thus, in conclusion

$$\begin{bmatrix} Vx' \\ Vy' \end{bmatrix} = \begin{bmatrix} \cos q & -\sin q \\ \sin q & \cos q \end{bmatrix} \begin{bmatrix} Vx \\ Vy \end{bmatrix}$$

Hilbert Space: Operators

- Conceptually, in the same way that

$$\begin{bmatrix} \cos q & -\sin q \\ \sin q & \cos q \end{bmatrix}$$

is determined by looking at the projections of $\hat{x}$ and $\hat{y}$ unit vectors under rotation, so are the elements of the linear transformation [H]. **Individually, we look at the projection of each basis function u_n, under the transformation H_{op}, on all basis functions u_m.** Mathematically this is formalized as the familiar

$$H_{nm} = \int d\vec{r}\, u_{m^*}(\vec{r})\left(H_{op} u_n(\vec{r})\right)$$

- Now lets look at changing coordinate systems. Given a function

$$\Phi(\vec{r}) = \sum_m f_m u_m(\vec{r})$$

written in a particular basis set.
If we were to change the basis set we could write the state-vector as:

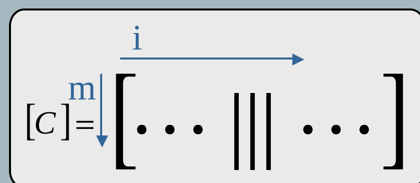
$$\Phi(\vec{r}) = \sum_i f_i' u_i'(\vec{r})$$

- This is done through a transformation matrix [C]

Hilbert Space: Changing Coordinates

38:30

- This matrix looks like



where the columns can be used to write u'_i as a linear combination of u_m's:

$$u'_i(\vec{r}) = \sum_m C_{mi} u_m(\vec{r})$$

- Once [C] is obtained, it can be used to transform operators from one basis set to another basis set.

- [C] can be fined by expressing the new basis set in terms of the old ones

$$\Phi(\vec{r}) = \sum_i f' u'_m(\vec{r})$$
$$= \sum_i f' \sum_m C_{mi} u_m(\vec{r})$$
$$= \sum_m u_m(\vec{r}) \sum_i C_{mi} f'_i$$
$$\therefore f_m = \sum_i C_{mi} f'_i$$

In matrix notation: $\{f\} = [C]\{f'\}$

Hilbert Space: Unitary Transformations

44:07

- Unitary Transformations are those which preserve the length of a vector, such that

$$\sum_m |f_m|^2 = \sum_i |f'_i|^2 \quad (1)$$

<u>In vector notation</u>

$$\{f\}^\dagger \{f\} = \{f'\}^\dagger \{f'\}$$

Note: "†" denotes the conjugate transpose.

- The claim is that the matrix that performs this type of transformation has to satisfy this condition:

$CC^\dagger = C^\dagger C = I$ But why?

- To see this we'll start from the left side of one and we'll try to get the right side using these relations:

$\{f\} = [C]\{f'\}$ and $\{f\}^\dagger = \{f'\}^\dagger [C]^\dagger$

We have: $\{f\}^\dagger \{f\} = \{f'\}^\dagger [C]^\dagger [C]\{f'\}$

The only way that the right side could be equal to the left is that:

$$[C]^\dagger [C] = I$$

- **Main points of this lecture:**
  - **Basis functions**
  - **Hilbert space**
  - **Dot product and orthogonality**
  - **Linear transformations and operators**
  - **Unitary transformations**