Set of square-integrable function L^2: function space F

Motivation:

• In our previous discussions we have seen that for free particles wave equations (Helmholtz or Schrödinger) can be expressed in terms of **eigenvalue equations**.
$H\phi(\vec{r}) = E\phi(\vec{r})$, or $\nabla^2 \vec{E} = -\omega^2 \mu\varepsilon \vec{E}$

• This approach is **more universal than the simple example given above**. For example, in the case of inhomogeneous but linear and isotropic medium such as **photonic crystals** the wave equation governing $\vec{H}(r)$ and $\vec{E}(r)$ can be written as

$\Theta\, \vec{H}(\vec{r}) = \left(\frac{\omega}{c}\right)^2 \vec{H}(\vec{r})$ and $\Xi\, \vec{E}(\vec{r}) = \left(\frac{\omega}{c}\right)^2 \vec{E}(\vec{r})$, where Θ **and** Ξ **are operators to be determined** (HW).

• In finding solutions to these eigenvalue equations one often has to expand the wave function $\psi(\vec{r})$ ($\phi, \vec{H}, \vec{E}$) in terms of other functions. Technically, this is **called projecting or expanding the wave function into a given function space**. You have already seen an example of this method in our discussion of wave packet and its spectrum decomposition.

$$\Psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} g(\vec{k})\, e^{i\vec{k}\cdot\vec{r} - i\omega t}\, dk_x dk_y dk_z \Rightarrow \psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} g(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, dk_x dk_y dk_z$$

with $g(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \psi(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}\, dk_x dk_y dk_z$

• In what follows we study the general properties of the function space, operators, and bases.

• If **wave function** $\Psi(r,t)$ is **square integrable** then

$$\iiint \left|\Psi(\vec{r},t)\right|^2 dr^3 < \infty \qquad (1)$$

• If (1) is satisfied then **we can always choose a multiplicative constant** for $\Psi(r,t)$ such that

$$\iiint \left|\Psi(\vec{r},t)\right|^2 dr^3 = 1 \qquad (1')$$

• If $\Psi(\vec{r},t)$ satisfies (1) or (1′) we say $\Psi(\vec{r},t)$ **is square-integrable**.

• **The set of square-integrable functions in mathematics is called** L^2 **set**.

• L^2 set has the structure of **Hilbert space**.

• We also assume that our wave packet $\Psi(\vec{r},t)$ **possess some regularity**. For example, we require that $\Psi(\vec{r},t)$ be **defined everywhere**, be **continuous everywhere**, and **differentiable**.

• Assigning the above physical meanings and constraints to $\Psi(\vec{r},t)$ implies that L^2 **set is too wide for our purposes**.

• We define the **function space** f **as a subset of** L^2; $\left(f \subset L^2\right)$ composed of sufficiently regular functions.

Linearity of function space f

• Let $\psi_1(\vec{r}) \in \{f\}$ and $\psi_2(\vec{r}) \in \{f\}$ then $\lambda_1\psi_1(\vec{r}) + \lambda_2\psi_2(\vec{r}) \in \{f\}$ where λ_1 and λ_2 are in general complex; $\lambda_1, \lambda_2 \in \{\underline{C}\}$. (HW)

Inner Product of Two Functions

• The **inner product** of two functions ϕ and ψ is defined by

$$(\phi,\psi) = \iiint \phi^*(\vec{r})\,\psi(\vec{r})\,dr^3 \tag{2}$$

• The following can be **shown to be true** (HW)

$$(\phi,\psi)^* = (\psi,\phi)$$

$$(\phi, \lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1(\phi,\psi_1) + \lambda_2(\phi,\psi_2)$$

$$(\phi_1\lambda_1 + \phi_2\lambda_2, \psi) = \lambda_1^*(\phi_1,\psi) + \lambda_2^*(\phi_2,\psi)$$

• Note that while $(\phi,\psi) = \iiint \phi^*(\vec{r})\,\psi(\vec{r})\,dr^3 \in \{\underline{C}\}$ **(is a complex number)**, for $\phi = \psi$ we have $(\psi,\psi) = \iiint \psi^*(\vec{r})\,\psi(\vec{r})\,dr^3 = \iiint |\psi(\vec{r})|^2\,dr^3 \in \{\Re\}$ **(is a positive real number)**

• $\sqrt{(\psi,\psi)}$ is called the **norm of** ψ.

• $(\psi,\psi) = \sqrt{(\psi,\psi)}\sqrt{(\psi,\psi)}$ is the **square of the norm**

• If $(\psi,\psi) = 0 \Rightarrow \psi = 0$. If $(\phi,\psi) = 0$ **we say** ϕ **and** ψ **are orthogonal**.

Schwartz Inequality

$\left|(\psi_1,\psi_2)\right| \le \underbrace{\sqrt{(\psi_1,\psi_1)}}_{\text{norm of }\psi_1}\underbrace{\sqrt{(\psi_2,\psi_2)}}_{\text{norm of }\psi_2}$. The Equality applies when $\psi_1 = \psi_2$

Operators

• **Operator** $\underline{A}$ **is a mathematical entity** which associates with any $\psi(\vec{r}) \in \{f\}$ another function $\psi'(\vec{r})$ that may or may not belong to $\{f\}$

$$\underline{A}\,\psi(\vec{r}) = \psi'(\vec{r}) \tag{1}$$

• Followings are examples of the operators

Parity $\underline{\Pi}$: $\underline{\Pi}\,\psi(x,y,z) = \psi(-x,-y,-z)$

Position $\underline{X}$: $\underline{X}\,\psi(x,y,z) = x\,\psi(x,y,z)$

Differential $\underline{D_x}$: $\underline{D_x}\,\psi(x,y,z) = \dfrac{\partial}{\partial x}\psi(x,y,z)$

• **Linear operator** is such an operator that satisfies the following:

$$\underline{A}\left[\lambda_1\psi_1(\vec{r}) + \lambda_2\psi_2(\vec{r})\right] = \lambda_1\underline{A}\,\psi_1(\vec{r}) + \lambda_2\underline{A}\,\psi_2(\vec{r})$$

Where $\lambda_1, \lambda_2 \in \{\underline{C}\}$

Commutators of two operators

• We define: $\underline{A}\,\underline{B}\left[\psi(\vec{r})\right] = \underline{A}\left[\underline{B}\,\psi(\vec{r})\right]$. In general $\underline{A}\,\underline{B} \ne \underline{B}\,\underline{A}$

• The **commutation of** $\underline{A}$ **and** $\underline{B}$ is defined as $[\underline{A},\underline{B}] = \underline{A}\,\underline{B} - \underline{B}\,\underline{A}$. Show that commutator operator for $\underline{X}$ and $\underline{D_x}$ is $-\underline{\mathbf{1}}$.

• You can think of $\psi(\vec{r})$ **as a vector and operator** $\underline{A}$ **as a matrix**.

Bases in vector function space

Discrete basis:

• Consider the **countable set of functions** $\{U_i(\vec{r})\}$, $i = 1, 2, \ldots, n, \ldots$, where $U_i \in \{f\}$. U_i is square integrable.

• The set $\{U_i(\vec{r})\}$ **is orthonormal if** $(U_i, U_j) = \iiint U_i^*(\vec{r}) U_j^*(\vec{r})\, dr^3 = \delta_{ij}$, where δ_{ij} is the **Kronecker delta** with $\delta_{ij} = 1$ for $i = j$, $\delta_{ij} = 0$ for $i \neq j$

• If every function $\psi(\vec{r}) \in \{f\}$ can be **expanded in one and only one way** in term of $U_i(\vec{r})$, given by

$$\psi(\vec{r}) = \sum_{i=1} c_i\, U_i(\vec{r}), \tag{1}$$

then we say the set $\{U_i(\vec{r})\}$ **constitute a basis**.

• When $\{U_i(\vec{r})\}$ **constitute a basis**, we sometime say that $\{U_i(\vec{r})\}$ is a **complete set of functions.**

• Note that from (1), $\psi(\vec{r})$ **is completely represented** in the $\{U_i(\vec{r})\}$ basis **by its coefficients of expansion**, i.e. c_i.

Coefficients of Expansion c_i

• The **coefficients of expansion** c_i are given by (HW)

$$c_i = (U_i, \psi) = \iiint dr^3 U_i^*(\vec{r})\, \psi(\vec{r}) \tag{2}$$

• In words, the coefficients of expansion are the **inner product of the wave function** $\psi(\vec{r})$ **and the bases functions.**

• Clearly the coefficients of expansion for $\psi(\vec{r})$ **on the basis** $\{U_i(\vec{r})\}$ **are in general different** from the coefficients of expansion for $\psi(\vec{r})$ **on another basis** $\{U_i'(\vec{r})\}$, i.e. $c_i \neq c_i'$, even though $\psi(\vec{r})$ is the same wave function.

• While a wave function $\psi(\vec{r})$ **can be expressed on a basis** $\{U_i(\vec{r})\}$ **in terms of series of complex number** (coefficients of expansion, c_i), the **operator** $\underline{A}$ **also can be expressed on the basis** $\{U_i(\vec{r})\}$ **in terms of series of numbers arranged in the form of a matrix**.

The inner product of two wave functions $\psi(\vec{r})$ and $\phi(\vec{r})$ in terms of their coefficients of expansion

• Let $\psi(\vec{r}) \in \{f\}$ and $\phi(\vec{r}) \in \{f\}$ **be expressed on the basis** $\{U_i(\vec{r})\}$ according to

$\psi(\vec{r}) = \sum_i c_i\, U_i(\vec{r})$ and $\phi(\vec{r}) = \sum_{j=1} b_j\, U_j(\vec{r})$, then

$$(\phi,\psi) = \left(\sum_j b_j\, U_j, \sum_i c_i\, U_i\right)$$

$$= \iiint \sum_j b_j^*\, U_j^* \sum_i c_i\, U_i dr^3$$

$$= \sum_i \sum_j \iiint b_j^* c_i\, U_j^*(\vec{r}) U_i(\vec{r})\, dr^3$$

$$= \sum_i \sum_j b_j^* c_i \iiint U_j^*(\vec{r}) U_i(\vec{r})\, dr^3 = \sum_i \sum_j b_j^* c_i\, (U_j, U_i)$$

$$= \sum_i \sum_j b_j^* c_i\, \delta_{ji} = \sum_i b_i^* c_i \Rightarrow$$

$$(\phi,\psi) = \sum_i b_i^* c_i$$

• For $\phi = \psi$ then $(\psi,\psi) = \sum_i c_i^* c_i = \sum_i |c_i|^2$

• One may draw **analogies between basis functions** $\{U_i(\vec{r})\}$ **and unit vectors in Cartesian coordinate** $\{\hat{e}_i\}$. For example, in Cartesian coordinates we have the basis vectors $\hat{e}_i, i = x, y, z \equiv (\hat{e}_x, \hat{e}_y, \hat{e}_z)$. Then note the following analogies:

Basis functions		**Unit vectors in Cartesian coordinates**
$(U_i, U_j) = \delta_{ij}$	$\Leftrightarrow$	$\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$; $i, j = x, y, z$
$\psi_i = \sum_{i=1} c_i U_i(\vec{r})$	$\Leftrightarrow$	$\vec{M} = \sum_{i=x,y,z} m_i \hat{e}_i$
$c_i = (U_i, \psi)$	$\Leftrightarrow$	$m_i = \hat{e}_i \cdot \vec{M}$
$(\phi,\psi) = \sum_i b_i^* c_i$	$\Leftrightarrow$	$\vec{M} \cdot \vec{N} = \sum_i \sum_j m_i n_j \hat{e}_i \cdot \hat{e}_j = \sum_i \sum_j m_i n_j \delta_{ij} = \sum_i m_i n_i$

Closure relation

• We have already seen the **orthonormality condition** for any two basis functions, i.e. $\iiint U_i^*(\vec{r}) U_j(\vec{r}) dr^3 = \delta_{ij}$.

• We now **establish a condition under which set** $\{U_i(\vec{r})\}$ **constitutes a basis; this condition is called closure relation.**

• For $\{U_i(\vec{r})\}$ to be a **basis (a complete set) we must be able to expand any function** $\psi(\vec{r})$ in the base, i.e.

$\psi(\vec{r}) = \sum_{i=1} c_i \, U_i(\vec{r})$, where $c_i = (U_i, \psi)$, then (1)

$$\psi(r) = \sum_i (U_i, \psi) U_i(\vec{r}) = \sum_i \left[\iiint U_i^*(\vec{r}\,') \, \psi(\vec{r}\,') \, dr'^3 \right] U_i(\vec{r}). \tag{2}$$

Interchanging $\sum$ and $\int$ we have

$$\psi(\vec{r}) = \iiint \psi(\vec{r}\,') dr'^3 \sum_i U_i^*(\vec{r}\,') U_i(\vec{r}). \tag{3}$$

For (3) to be true $\sum_i U_i^*(\vec{r}\,') U_i(\vec{r})$ **must have the form** $\delta(\vec{r}\,' - \vec{r}) = \delta(\vec{r} - \vec{r}\,')$

• Therefore, the **closure relation can be written as**

$\sum U_i(\vec{r}) U_i^*(\vec{r}\,') = \delta(\vec{r} - \vec{r}\,')$ (Closure relation) (4)

• **Conversely if (4) is satisfied (1) is always true**, because

$$\psi(\vec{r}) = \iiint dr'^3 \delta(\vec{r} - \vec{r}\,') \psi(\vec{r}\,') = \iiint dr'^3 \sum_i U_i^*(\vec{r}\,') U_i(\vec{r}) \psi(\vec{r}\,'). \tag{5}$$

Interchanging $\sum$ and $\int$ order and following the above procedure in reverse **we will obtain** $\psi(\vec{r}) = \sum_i c_i \, U_i(\vec{r})$.

Summary

• **Orthonormality condition** is given by $(U_i, U_j) = \iiint dr^3 \, U_i^*(\vec{r}) U_j(\vec{r}) = \delta_{ij}$

• **Closure relation** is given by $\sum U_i^*(\vec{r}\,') U_i(\vec{r}) = \delta(\vec{r} - \vec{r}\,')$

• Note **orthonormality involves bases with different indices** i **and** j**, but the same argument** $(\vec{r})$; however **closure involves bases with the same index** i**, but different arguments** $\vec{r}$ **and** $\vec{r}\,'$**.**

Bases that do not belong to the function space $\{f\}$: (bases that are not square-integrable)

• So far we have studied bases that were square-integrable, i.e. $U_i(\vec{r}) \in \{f\}$, **here we relax this condition and consider bases that** $\notin L^2$. We will generalize our results for expanding the wave function $\psi(\vec{r})$ on such bases and **will find the coefficients of expansion, the orthonormality, and closure conditions**.

• We start our study with the familiar case of **Fourier transform and plane wave basis**.

Bases of Plane Waves and Fourier Transform – The One Dimensional Case

• Consider the well known **Fourier pair**

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \overline{\psi}(k)\, e^{ikx} dk \qquad (1)$$

$$\overline{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x)\, e^{-ikx} dx \qquad (2)$$

• Functions $V_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}$ (plane waves) **form a set** $\{V_k(x)\}$ for **which the index** k **is continuous.**

• Note that integral of $|V_k(x)|^2 = \frac{1}{2\pi}$ over x diverges $\Rightarrow V_k(x)$ **is not square-integrable**. Also whereas for $\{U_i(x)\}$, i was discrete for $\{V_k(x)\}$, k **is continuous**.

Expansion of wave function $\psi(x)$ on $\{V_k(x)\}$ basis

• **We write (1) and (2) as**

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \overline{\psi}(k)\, e^{ikx} dk = \int \overline{\psi}(k) V_k(x)\, dk \text{ with } V_k = \frac{e^{ikx}}{\sqrt{2\pi}}\text{, and} \qquad (3)$$

$$\overline{\psi}(k) = \int \psi(x) \frac{1}{\sqrt{2\pi}} e^{-ikx} dx = \int V_k^* \, \psi(x)\, dx = (V_k, \psi) \qquad (4)$$

• **Comparing the above continuous basis with our previous discrete basis** we see

$$\psi(x) = \int \overline{\psi}(k) V_k(x)\, dk \qquad \Leftrightarrow \qquad \psi(x) = \sum_{i=1} c_i \, U_i(x) \text{ and}$$

$$\overline{\psi}(k) = \int V_k^* \, \psi(x)\, dx = (V_k, \psi) \qquad \Leftrightarrow \qquad c_i = \int dx\, U_i^*(x) \psi(x) = (U_i, \psi)$$

• $\overline{\psi}(k)$ **is the coefficient of expansion for** $\psi(x)$ **in the** $\{V_k(x)\}$ **basis**. This coefficient of expansion can be found from the inner product of ψ and the basis functions V_k.

$\{V_k\} \Leftrightarrow \{U_i\}$

$\int \Leftrightarrow \sum$

$k \equiv$ continuous $\Leftrightarrow$ $i \equiv$ discrete

Norm (square of the norm) of the function $\psi(x)$

• Recall $(\psi,\psi) = \int \psi^*(x)\,\psi(x)\,dx$

• From **Parseval's theorem** (HW) it can be shown

$$(\psi,\psi) = \int \psi^*(x)\,\psi(x)\,dx = \int |\psi(x)|^2\,dx = \int \overline{\psi}^*(k)\,\overline{\psi}(k)\,dk = \int \left|\overline{\psi}(k)\right|^2 dk$$

• **Compare** $(\psi,\psi) = \int \left|\overline{\psi}(k)\right|^2 dk$ **with** $(\psi,\psi) = \sum_i |c_i|^2$ for discrete basis.

Orthonormalization

• For the basis $\{V_k(x)\}$ the **orthonormalization** is given by (HW)

$$(V_k, V_{k'}) = \int V_k^*(x) V_{k'}(x)\,dx = \delta(k-k')$$

• **Compare this to** $(U_i, U_j) = \int U_i^*(x) U_j(x)\,dx = \delta_{ij}$ for $\{U_i(x)\}$ basis.

• Orthonormalization for $\{V_k(x)\}$ results in **Dirac-Delta function** where as for $\{U_i(x)\}$ basis it results in **Kronecker delta function**.

• Note that

$$(V_k, V_{k'}) = \delta(k-k') \Rightarrow (V_k, V_{k'})^* = \delta^*(k-k') \Rightarrow$$
$$(V_{k'}, V_k) = \delta(k-k') \Rightarrow (V_k, V_{k'}) = (V_{k'}, V_k)$$

Closure relation for $\{V_k(x)\}$

• For $\{V_k\}$ it can be shown that **closure relation is given by** (HW)

$\int V_k(x) V_k^*(x')\,dk = \delta(x-x')$.

Since $[\delta(x-x')]^* = \delta(x-x') = \delta(x'-x)$ then we can write

$\int V_k(x) V_k^*(x')dk = \int V_k^*(x) V_k(x')dk = \delta(x-x') = \delta(x'-x)$ (Closure relation)

• **Compare** the $\int V_k(x) V_k^*(x')\,dk = \delta(x-x')$ **for continuous basis with** $\sum_i U_i(x) U_i^*(x') = \delta(x-x')$ **for discrete basis**.

Extension to Three Dimensions

• In **three dimensions** the plane wave basis is given by $\{V_k(\vec{r})\}$ where $V_k(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$

• **Expansion of the wave function** is given by

$$\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \iiint \overline{\psi}(\vec{k}) e^{i\vec{k}\cdot\vec{r}} dk^3 = \iiint dk^3 \overline{\psi}(\vec{k}) V_k(\vec{r})$$

• **Coefficients of expansions** are

$$\overline{\psi}(\vec{k}) = (V_k, \psi) = \iiint dr^3 V_k^*(\vec{r}) \psi(\vec{r})$$

• **Inner product** is given by

$$(\phi, \psi) \equiv \iiint \phi^*(\vec{r}) \psi(\vec{r}) dr^3 = \iiint \overline{\phi}^*(\vec{k}) \overline{\psi}(\vec{k}) dk^3$$

• **Orthonormality** condition is given by

$$(V_k, V_{k'}) = (V_{k'}, V_k) = \delta(\vec{k} - \vec{k}') = \delta(\vec{k}' - \vec{k})$$

• **Closure condition** is given by

$$\iiint V_k(\vec{r}) V_k^*(\vec{r}') dk^3 = \iiint V_k^*(\vec{r}) V_k(\vec{r}') dk^3 = \delta(\vec{r} - \vec{r}') = \delta(\vec{r}' - \vec{r})$$

Delta functions as basis

• Using the properties of Dirac-Delta function we have

$$\psi(r) = \iiint dr_0^3 \psi(\vec{r}_0) \delta(\vec{r} - \vec{r}_0) \quad (1)$$

and

$$\psi(\vec{r}_0) = \iiint dr^3 \, \psi(\vec{r}) \delta(\vec{r}_0 - \vec{r}). \quad (2)$$

Where $\vec{r}_0$ stands for (x_0, y_0, z_0) and $\vec{r}$ for (x, y, z) and $\delta(\vec{r} - \vec{r}_0) = \delta(x - x_0)\delta(y - y_0)\delta(z - z_0)$.

• Let us define **basis** $\{\xi_{r_0}(\vec{r})\}$ **where** $\xi_{r_0}(\vec{r}) = \delta(\vec{r} - \vec{r}_0)$

• Note that $\xi_{r_0}(\vec{r}) \notin L^2$

Expansion of Function $\psi(\vec{r})$ on the Basis $\{\xi_{r_0}(\vec{r})\}$

• $\psi(r) = \iiint dr_0^{\,3} \psi(\vec{r}_0)\,\delta(\vec{r} - \vec{r}_0) \;\Rightarrow\; \psi(\vec{r}) = \iiint dr_0^{\,3}\; \psi(\vec{r}_0)\,\xi_{r_0}(\vec{r})$, where $\xi_{r_0}(\vec{r}) = \delta(\vec{r} - \vec{r}_0)$.
Compare these results with $\psi(\vec{r}) = \sum_i c_i\, U_i(\vec{r})$ (1)

Coefficients of Expansion

• $\psi(\vec{r}_0) = \iiint dr^3\; \psi(\vec{r})\,\delta(\vec{r}_0 - \vec{r}) \;\Rightarrow\; \psi(r_0) = \iiint dr^3\; \xi^*_{r_0}(\vec{r})\,\psi(\vec{r}) = (\xi_{r_0}, \psi)$, where $\xi^*_{r_0}(\vec{r}) = \delta^*(\vec{r} - \vec{r}_0) = \delta(\vec{r} - \vec{r}_0) = \delta(\vec{r}_0 - \vec{r})$. Compare these coefficients of expansion with the discrete set $c_i = \iiint dr^3\; U_i^*(\vec{r})\,\psi(\vec{r}) = (U_i, \psi)$

• **Note that coefficients of expansion for** $\psi(\vec{r})$ **on the basis** $\{\xi_{r_0}(\vec{r})\}$ **are the values of** $\psi(r)$ **at each point in space.**

• $\psi(\vec{r}_0)$ **is similar to** c_i but **where** r_0 **is a continuous index** for $\{\xi_{r_0}(\vec{r})\}$ basis, i is a discrete index for $\{U_i(\vec{r})\}$ basis.

Inner Product for $\{\xi_{r_0}(\vec{r})\}$

$(\phi, \psi) = \iiint \phi^*(\vec{r}_0)\,\psi(\vec{r}_0)\, dr_0^{\,3}$. **Note this is in fact the definition of the inner product**.
Compare the above to $(\phi, \psi) = \sum_i b_i^* c_i$.

Orthonormality

$(\xi_{r_0}, \xi_{r_0'}) = \iiint \delta(\vec{r} - \vec{r}_0)\,\delta(\vec{r} - \vec{r}_0')\, dr^3 = \delta(\vec{r}_0 - \vec{r}_0') = \delta(\vec{r}_0' - \vec{r}_0)$. Compare this to
$(U_i, U_j) = \iiint U_i^*(\vec{r})\, U_j(\vec{r})\, dr^3 = \delta_{ij}$

Closure relation

$\iiint \xi_{r_0}(\vec{r})\, \xi^*_{r_0}(\vec{r}')\, dr_0^{\,3} = \iiint \delta(\vec{r} - \vec{r}_0)\,\delta(\vec{r}_0 - \vec{r}')dr_0^{\,3} = \delta(\vec{r} - \vec{r}')$.
Compare this to $\sum_i U_i(\vec{r})\,U_i^*(\vec{r}') = \delta(\vec{r} - \vec{r}')$

Continuous orthonormal bases: generalization

• We can **generalize our results** obtained for $\{V_k(\vec{r})\}$ and $\{\xi_{r_0}(\vec{r})\}$ by introducing the **continuous orthonormal basis** $\{W_\alpha(\vec{r})\}$ which is a set of function $W_\alpha(\vec{r})$ **labeled with the continuous index** α . The basis $\{W_\alpha(\vec{r})\}$ will satisfy the following

Expansion of wave function	$\psi(r) = \iiint d\alpha^3 \; c(\alpha) W_\alpha(\vec{r})$	$\Leftrightarrow$	$\psi(r) = \sum_i c_i \, U_i(\vec{r})$
Coefficients of Expansion	$c(\alpha) = (W_\alpha, \psi) = \iiint dr^3 \; W_\alpha^*(\vec{r}) \psi(\vec{r})$	$\Leftrightarrow$	$c_i = (U_i, \psi) = \iiint dr^3 \; U_i^*(\vec{r}) \psi(\vec{r})$
Scalar product	$(\phi, \psi) = \iiint d\alpha^3 \; b^*(\alpha) c(\alpha)$	$\Leftrightarrow$	$(\phi, \psi) = \sum b_i^* c_i$
Square of the norm	$(\psi, \psi) = \iiint d\alpha^3 \; \lvert c(\alpha) \rvert^2$	$\Leftrightarrow$	$(\psi, \psi) = \sum_i \lvert c_i \rvert^2$
Orthonormalization relation	$(W_\alpha, W_{\alpha'}) = \iiint dr^3 W_\alpha(\vec{r}) W_{\alpha'}(\vec{r}) = \delta(\alpha - \alpha')$	$\Leftrightarrow$	$(U_i, U_j) = \delta_{ij}$
Closure relation	$\iiint d\alpha^3 \; W_\alpha(\vec{r}) W_\alpha^*(\vec{r}') = \delta(\vec{r} - \vec{r}')$	$\Leftrightarrow$	$\sum U_i(\vec{r}) U_i^*(\vec{r}') = \delta(\vec{r} - \vec{r}')$