Chapter 5
Vector Spaces

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August 2021

5.1 Vectors in Function Spaces

5.1.1 If there are two expansions of $f(x)$, so

$$f(x) = \sum_{n=0}^{\infty} a_n \varphi_n(x) = \sum_{n=0}^{\infty} b_n \varphi_n(x)$$

then

$$g(x) = \sum_{n=0}^{\infty} (a_n - b_n)\varphi_n(x) = 0$$

$$\langle g(x)|g(x)\rangle = \sum_{n=0}^{\infty} (a_n - b_n)^2 = 0$$

so $a_n = b_n$, and the expansion is unique.

5.1.2 If

$$f(x) = \sum_{i=1}^{N} c_i \varphi_i(x) = \sum_{i=1}^{N} c_i' \varphi_i(x)$$

so

$$\sum_{i=1}^{N} (c_i - c_i')\varphi_i(x)$$

By definition of linear independence, the linear combination of a linear independent set equals zero only if all the coefficient is zero. The set of φ_i is linear independent, so $c_i - c_i'$ must be zero, which means $c_i = c_i'$, the components are unique.

5.1.3 The mean square error M is

$$M = \int_0^1 (f(x) - \sum_j c_j x^j)^2 dx$$

$$= \int_0^1 \left[f(x)^2 + (\sum_j c_j x^j)(\sum_j c_j x^j) - 2f(x)(\sum_j c_j x^j) \right] dx$$

When M is minimized, $\frac{\partial M}{\partial c_i} = 0$ for every i, so

$$\frac{\partial M}{\partial c_i} = \int_0^1 \left[2x^i(\sum_j c_j x^j) - 2f(x)x^i \right] dx = 0$$

so

$$\sum_j \int_0^1 x^{i+j} dx \cdot c_j = \int_0^1 x^i f(x) dx$$

Let $\int_0^1 x^{i+j} dx = A_{ij}, \quad \int_0^1 x^i f(x) dx = b_i$, then the equation becomes

$$\sum_j A_{ij} c_j = b_i$$

or A$\mathbf{c} = \mathbf{b}$ in matrix form.

5.1.4 Let $F(x) = \varphi_i(x)$, then

$$a_j = \delta_{ij} = \int_a^b \varphi_i(x)\varphi_j(x)w(x)dx$$

so the basis are orthonormal.

When the mean square error is minimized,

$$\frac{\partial}{\partial c_n}\left(\int_a^b [F(x) - \sum_{k=o}^{m} c_k\varphi_k(x)]^2 w(x)dx\right) = 0$$

so

$$\int_a^b 2[F(x) - \sum_{k=o}^{m} c_k\varphi_k(x)](-\varphi_n(x))w(x)dx = 0$$

$$-\int_a^b F(x)\varphi_n(x)w(x)dx + \sum_{k=0}^{m} c_k\delta_{kn} = 0$$

Note that the first term is $-a_n$, and the second term is c_n, so

$$c_n = a_n$$

5.1.5 (a)

$$\int_{-\pi}^{\pi} \frac{\sin(2n+1)x}{2n+1}\frac{\sin(2m+1)x}{2m+1}dx = \int_{-\pi}^{\pi} \frac{\cos(2(n-m)x) - \cos(2(n+m+1)x)}{2(2n+1)(2m+1)}$$

$$= \begin{cases} 0, & when\ n \neq m \\ \frac{\pi}{(2n+1)^2}, & when\ n = m \end{cases}$$

so

$$\int_{-\pi}^{\pi} [f(x)]^2\, dx = \int_{-\pi}^{\pi} \frac{4h^2}{\pi^2}(\sum_{n=0}^{\infty}\frac{\sin(2n+1)x}{2n+1})(\sum_{m=0}^{\infty}\frac{\sin(2m+1)x}{2m+1})dx$$

$$= \frac{4h^2}{\pi^2}\sum_{n=0}^{\infty}\frac{\pi}{(2n+1)^2} = \frac{4h^2}{\pi}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}$$

(b)

$$\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2} = \frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \frac{1}{7^2} + \cdots$$

$$= (\frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \frac{1}{5^2} + \frac{1}{6^2} + \frac{1}{7^2} + \cdots) - \frac{1}{2^2}(\frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \cdots)$$

$$= \frac{3}{4}\zeta(2) = \frac{\pi^2}{8}$$

so

$$\frac{4h^2}{\pi}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2} = \frac{4h^2}{\pi}\frac{\pi^2}{8} = \frac{\pi}{2}h^2$$

5.1.6

$$\left[\int_a^b f(x)g(x)dx\right]^2 + \frac{1}{2}\int_a^b dx \int_a^b dy\,[f(x)g(y)-f(y)g(x)]^2 = \int_a^b [f(x)]^2\,dx \int_a^b [g(x)]^2\,dx$$

and note that $\frac{1}{2}\int_a^b dx \int_a^b dy\,[f(x)g(y)-f(y)g(x)]^2 \geq 0$, so

$$\left[\int_a^b f(x)g(x)dx\right]^2 \leq \int_a^b [f(x)]^2\,dx \int_a^b [g(x)]^2\,dx$$

To prove the identity, note that

$$\frac{1}{2}\int_a^b dx \int_a^b dy\,[f(x)g(y)-f(y)g(x)]^2 = \frac{1}{2}\int_a^b dx \int_a^b dy\,\left[f(x)^2g(y)^2 + f(y)^2g(x)^2 - 2f(x)g(x)f(y)g(y)\right]$$

$$= \frac{1}{2}\int_a^b dx\left[f(x)^2\int_a^b [g(y)]^2dy + (\int_a^b [f(y)]^2dy)\;g(x)^2 - 2f(x)g(x)\int_a^b f(y)g(y)dy\right]$$

$$= \frac{1}{2}\left[\int_a^b [f(x)]^2dx\int_a^b [g(y)]^2dy + \int_a^b [f(y)]^2dy\int_a^b [g(x)]^2dx - 2\int_a^b f(x)g(x)dx\int_a^b f(y)g(y)dy\right]$$

$$= \int_a^b [f(x)]^2dx\int_a^b [g(x)]^2dx - \left[\int_a^b f(x)g(x)dx\right]^2$$

Rearranging the terms we get the identity.

5.1.7 The basis are orthonormal, so $\langle a_i\varphi_i|a_j\varphi_j\rangle$ is zero when $i\neq j$ and is $|a_i|^2$ when $i=j$. Let $f=\sum_k a_k\varphi_k$, k can be infinite, and let $\sum_n a_n\varphi_n$ be an incomplete expansion of f, then

$$I = \left\langle f - \sum_n a_n\varphi_n \middle| f - \sum_n a_n\varphi_n\right\rangle$$

$$= \langle f|f\rangle - \left\langle \sum_n a_n\varphi_n \middle| f\right\rangle - \left\langle f \middle| \sum_n a_n\varphi_n\right\rangle + \left\langle \sum_n a_n\varphi_n \middle| \sum_n a_n\varphi_n\right\rangle$$

$$= \langle f|f\rangle - \left\langle \sum_n a_n\varphi_n \middle| \sum_k a_k\varphi_k\right\rangle - \left\langle \sum_k a_k\varphi_k \middle| \sum_n a_n\varphi_n\right\rangle + \left\langle \sum_n a_n\varphi_n \middle| \sum_n a_n\varphi_n\right\rangle$$

$$= \langle f|f\rangle - \sum_n |a_n|^2 - \sum_n |a_n|^2 + \sum_n |a_n|^2$$

$$= \langle f|f\rangle - \sum_n |a_n|^2 \geq 0$$

so

$$\langle f|f\rangle \geq \sum_n |a_n|^2$$

5.1.8 By integrating by parts, we have

$$\int_0^1 \sin\pi x\,dx = \frac{\pi}{2}$$

$$\int_0^1 x\sin\pi x\,dx = \frac{1}{\pi} - \frac{1}{\pi}\int_0^1 \cos\pi x\,dx = \frac{1}{\pi}$$

$$\int_0^1 x^2\sin\pi x\,dx = \frac{1}{\pi} - \frac{2}{\pi^2}\int_0^1 \sin\pi x\,dx = \frac{1}{\pi} - \frac{4}{\pi^3}$$

$$\int_0^1 x^3 \sin \pi x \, dx = \frac{1}{\pi} - \frac{6}{\pi^2} \int_0^1 x \sin \pi x \, dx = \frac{1}{\pi} - \frac{6}{\pi^3}$$

Let $\sin \pi x = \sum a_n \varphi_n$, then

$$a_0 = \frac{\langle \varphi_0 | \sin \pi x \rangle}{\langle \varphi_0 | \varphi_0 \langle} = \frac{I_0}{1} = \frac{2}{\pi}$$

$$a_1 = \frac{\langle \varphi_1 | \sin \pi x \rangle}{\langle \varphi_1 | \varphi_1 \rangle} = \frac{2I_1 - I_0}{\frac{1}{3}} = 0$$

$$a_2 = \frac{\langle \varphi_2 | \sin \pi x \rangle}{\langle \varphi_2 | \varphi_2 \rangle} = \frac{6I_2 - 6I_1 + I_0}{\frac{1}{5}} = \frac{10}{\pi} - \frac{120}{\pi^3}$$

$$a_3 = \frac{\langle \varphi_3 | \sin \pi x \rangle}{\langle \varphi_3 | \varphi_3 \rangle} = \frac{20I_3 - 30I_2 + 12I_1 - I_0}{\frac{1}{7}} = 0$$

so

$$\sin \pi x = \frac{2}{\pi}\varphi_0 + (\frac{10}{\pi} - \frac{120}{\pi^3})\varphi_2 + \cdots$$

5.1.9 Integrating by parts for n times, we have

$$\int_0^\infty x^n e^{-2x} dx = \frac{n!}{2^{n+1}}$$

Let $e^{-x} = \sum a_n L_n(x)$, then

$$a_0 = \langle L_0 | e^{-x} \rangle = \int_0^\infty e^{-2x} dx = \frac{1}{2}$$

$$a_1 = \langle L_1 | e^{-x} \rangle = \int_0^\infty e^{-2x} dx - \int_0^\infty x e^{-2x} dx = \frac{1}{4}$$

$$a_2 = \langle L_2 | e^{-x} \rangle = \int_0^\infty e^{-2x} dx - 2\int_0^\infty x e^{-2x} dx + \frac{1}{2}\int_0^\infty x^2 e^{-2x} dx = \frac{1}{8}$$

$$a_3 = \langle L_3 | e^{-x} \rangle = \int_0^\infty e^{-2x} dx - 3\int_0^\infty x e^{-2x} dx + \frac{3}{2}\int_0^\infty x^2 e^{-2x} dx - \frac{1}{6}\int_0^\infty x^3 e^{-2x} dx = \frac{1}{16}$$

so

$$e^{-x} = \frac{1}{2}L_0 + \frac{1}{4}L_1 + \frac{1}{8}L_2 + \frac{1}{16}L_3 + \cdots$$

5.1.10 Expand φ_n in the χ_n basis, we have

$$\varphi_n = \sum_m \chi_m \langle \chi_m | \varphi_n \rangle$$

so

$$f = \sum_n \varphi_n a_n = \sum_n \sum_m \chi_m \langle \chi_m | \varphi_n \rangle a_n$$

5.1.11

$$\sum_j |\hat{\mathbf{e}}_j\rangle \langle \hat{\mathbf{e}}_j | \mathbf{a} \rangle = \sum_j \hat{\mathbf{e}}_j (\hat{\mathbf{e}}_j \cdot \mathbf{a}) = \mathbf{a}$$

5.1.12

$$\langle \mathbf{a} | \mathbf{a} \rangle = a_1^2 - 2a_1a_2 + ka_2^2 = (a_1 - a_2)^2 + (k-1)a_2^2 > 0 \quad \textit{(when } \mathbf{a} \neq 0\textit{)}$$

so $k - 1 > 0$, $k > 1$.

$$\langle \mathbf{a} | \mathbf{b} \rangle^* = a_1b_1 - a_1b_2 - a_2b_1 + ka_2b_2 = b_1a_1 - b_1a_2 - b_2a_1 + kb_2a_2 = \langle \mathbf{b} | \mathbf{a} \rangle$$

$$\langle \mathbf{a} | \mathbf{b} + \mathbf{b}' \rangle = a_1(b_1 + b_1') - a_1(b_2 + b_2') - a_2(b_1 + b_1') + ka_2(b_2 + b_2')$$
$$= (a_1b_1 - a_1b_2 - a_2b_1 + ka_2b_2) + (a_1b_1' - a_1b_2' - a_2b_1' + ka_2b_2') = \langle \mathbf{a} | \mathbf{b} \rangle + \langle \mathbf{a} | \mathbf{b}' \rangle$$

$$\langle \mathbf{a} | x\mathbf{b} \rangle = a_1xb_1 - a_1xb_2 - a_2xb_1 + ka_2xb_2 = x(a_1b_1 - a_1b_2 - a_2b_1 + ka_2b_2) = x\langle \mathbf{a} | \mathbf{b} \rangle$$

so the condition for the scalar product to be valid is $k > 1$.

5.2 Gram-Schmidt Orthogonalization

5.2.1

$$P_0^*(x) = 1$$

$$\psi_1(x) = x - 1\frac{\langle 1|x\rangle}{\langle 1|1\rangle} = x - \frac{\int_0^1 x dx}{\int_0^1 dx} = x - \frac{1}{2}$$

$$P_1^*(x) = \frac{\psi_1(x)}{\psi_1(1)} = 2x - 1$$

$$\psi_2(x) = x^2 - 1\frac{\langle 1|x^2\rangle}{\langle 1|1\rangle} - (2x-1)\frac{\langle 2x-1|x^2\rangle}{\langle 2x-1|2x-1\rangle} = x^2 - \frac{\int_0^1 x^2 dx}{\int_0^1 dx} - (2x-1)\frac{\int_0^1 (2x^3 - x^2)dx}{\int_0^1 (2x-1)^2 dx} = x^2 - x + \frac{1}{6}$$

$$P_2^*(x) = \frac{\psi_2(x)}{\psi_2(1)} = 6x^2 - 6x + 1$$

$$\psi_3(x) = x^3 - 1\frac{\langle 1|x^3\rangle}{\langle 1|1\rangle} - (2x-1)\frac{\langle 2x-1|x^3\rangle}{\langle 2x-1|2x-1\rangle} - (6x^2-6x+1)\frac{\langle 6x^2-6x+1|x^3\rangle}{\langle 6x^2-6x+1|6x^2-6x+1\rangle} = x^3 - \frac{3}{2}x^2 + \frac{3}{5}x - \frac{1}{20}$$

$$P_3^*(x) = \frac{\psi_3(x)}{\psi_3(1)} = 20x^3 - 30x^2 + 12x - 1$$

5.2.2

$$\varphi_0 = 1$$

$$L_0 = \frac{\varphi_0}{\langle \varphi_0|\varphi_0\rangle^{1/2}} = \frac{1}{(\int_0^\infty e^{-x}dx)^{1/2}} = \pm 1 \quad (\textit{choose } 1)$$

$$\varphi_1 = x - 1\int_0^\infty 1xe^{-x}dx = x - 1$$

$$L_1 = \frac{\varphi_1}{\langle \varphi_1|\varphi_1\rangle^{1/2}} = \frac{x-1}{(\int_0^\infty (x-1)^2 e^{-x}dx)^{1/2}} = \pm(x-1) \quad (\textit{choose } -x+1)$$

$$\varphi_2 = x^2 - 1\int_0^\infty 1x^2e^{-x}dx - (1-x)\int_0^\infty (1-x)x^2e^{-x}dx = x^2 - 4x + 2$$

$$L_2 = \frac{\varphi_2}{\langle \varphi_2|\varphi_2\rangle^{1/2}} = \frac{x^2-4x+2}{(\int_0^\infty (x^2-4x+2)^2e^{-x}dx)^{1/2}} = \pm\frac{x^2-4x+2}{2} \quad (\textit{choose } \frac{x^2-4x+2}{2})$$

(The choice of sign in the normalization is arbitrary and is so chosen to match the answer given in the text.)

5.2.3

$$\psi_0(x) = 1$$

$$\varphi_0(x) = \frac{\psi_0}{\langle \psi_0|\psi_0\rangle^{1/2}} = \frac{1}{(\int_0^\infty xe^{-x}dx)^{1/2}} = 1$$

$$\psi_1(x) = x - 1\int_0^\infty 1x\cdot xe^{-x}dx = x - 2$$

$$\varphi_1(x) = \frac{\psi_1}{\langle \psi_1|\psi_1\rangle^{1/2}} = \frac{x-2}{(\int_0^\infty (x^2-4x+4)xe^{-x}dx)^{1/2}} = \frac{x-2}{\sqrt{2}}$$

$$\psi_2(x) = x^2 - 1\int_0^\infty 1x^2\cdot xe^{-x}dx - \frac{x-1}{\sqrt{2}}\int_0^\infty \frac{x-2}{\sqrt{2}}x^2\cdot xe^{-x}dx = x^2 - 6x + 6$$

$$\varphi_2(x) = \frac{\psi_2}{\langle \psi_2|\psi_2\rangle^{1/2}} = \frac{x^2-6x+6}{(\int_0^\infty (x^4-12x^3+48x^2-72x+36)xe^{-x}dx)^{1/2}} = \frac{x^2-6x+6}{2\sqrt{3}}$$

(using the formula $\int_0^\infty x^n e^{-x}dx = n!$ can facilate the calculation.)

5.2.4 To calculate the scalar product, we need the Gaussian integral $\int_{-\infty}^{\infty} x^n e^{-x^2} dx$. When n is odd, $\int_{-\infty}^{\infty} x^n e^{-x^2} dx = 0$ because $x^n e^{-x^2}$ is odd function. When n is even, from Example 1.10.7 we have $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$, and by substitution we have

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \frac{\sqrt{\pi}}{\sqrt{a}}$$

differentiate both sides regarding a,

$$\frac{d}{da}\int_{-\infty}^{\infty} e^{-ax^2} dx = \int_{-\infty}^{\infty} (-x^2) e^{-ax^2} dx = -\frac{1}{2}\frac{\sqrt{\pi}}{a^{-\frac{3}{2}}}$$

so

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{-\frac{3}{2}}}$$

differentiate again,

$$\frac{d}{da}\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \int_{-\infty}^{\infty} (-x^4) e^{-ax^2} dx = -\frac{3}{4}\frac{\pi}{a^{-\frac{5}{2}}}$$

so

$$\int_{-\infty}^{\infty} x^4 e^{-ax^2} dx = \frac{3\sqrt{\pi}}{4a^{-\frac{3}{2}}}$$

Let φ_n be the non-scaled function, and $H_n = a_n \varphi_n$, so $\langle H_n | H_n \rangle = \int_{-\infty}^{\infty} a_n^2 \varphi_n^2 e^{-x^2} dx = 2^n n! \sqrt{\pi}$. Then

$$\varphi_0 = 1$$

$$\langle H_0 | H_0 \rangle = \int_{-\infty}^{\infty} a_0^2 1^2 e^{-x^2} dx = a_0^2 \sqrt{\pi} = \sqrt{\pi}$$

so $a_0 = 1$, and $H_0 = 1$.

$$\varphi_1 = x - 1\frac{\int_{-\infty}^{\infty} 1 \cdot x e^{-x^2} dx}{\int_{-\infty}^{\infty} 1 \cdot 1 e^{-x^2} dx} = x$$

$$\langle H_1 | H_1 \rangle = \int_{-\infty}^{\infty} a_1^2 x^2 e^{-x^2} dx = a_1^2 \frac{\sqrt{\pi}}{2} = 2\sqrt{\pi}$$

so $a_1 = 2$, and $H_1 = 2x$.

$$\varphi_2 = x^2 - 1\frac{\int_{-\infty}^{\infty} 1 \cdot x^2 e^{-x^2} dx}{\int_{-\infty}^{\infty} 1 \cdot 1 e^{-x^2} dx} - 2x\frac{\int_{-\infty}^{\infty} 2x \cdot x^2 e^{-x^2} dx}{\int_{-\infty}^{\infty} 2x \cdot 2x e^{-x^2} dx} = x^2 - \frac{1}{2}$$

$$\langle H_2 | H_2 \rangle = \int_{-\infty}^{\infty} a_2^2 (x^2 - \frac{1}{2})^2 e^{-x^2} dx = a_2^2 \frac{\sqrt{\pi}}{2} = 8\sqrt{\pi}$$

so $a_2 = 4$, and $H_2 = 4x^2 - 2$.

5.2.5

$$\int_{-1}^{1} \frac{x^{2n}}{\sqrt{1-x^2}} dx = \begin{cases} \pi, & n = 0 \\ \pi\frac{(2n-1)!!}{(2n)!!}, & n = 1, 2, 3 \cdots \end{cases}$$

from Exercise 13.3.2, and $\int_{-1}^{1} \frac{x^{2n+1}}{\sqrt{1-x^2}} dx = 0$ because $\frac{x^{2n+1}}{\sqrt{1-x^2}}$ is an odd function.

Let φ_n be the non-scaled function, and $T_n = a_n \varphi_n$, so $\langle T_n | T_n \rangle = \int_{-1}^{1} a_n^2 \varphi_n^2 \frac{1}{\sqrt{1-x^2}} dx$. Then

$$\varphi_0 = 1$$

$$\langle T_0 | T_0 \rangle = \int_{-1}^{1} a_0^2 \frac{1}{\sqrt{1-x^2}} dx = a_0^2 \pi = \pi$$

so $a_0 = 1$, and $T_0 = 1$.

$$\varphi_1 = x - 1\frac{\int_{-1}^{1} 1 \cdot x \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} 1 \cdot 1 \frac{1}{\sqrt{1-x^2}} dx} = x$$

$$\langle T_1 | T_1 \rangle = \int_{-1}^{1} a_1^2 x^2 \frac{1}{\sqrt{1-x^2}} dx = a_1^2 \frac{\pi}{2} = \frac{\pi}{2}$$

so $a_1 = 1$, and $T_1 = x$.

$$\varphi_2 = x^2 - 1\frac{\int_{-1}^{1} 1 \cdot x^2 \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} 1 \cdot 1 \frac{1}{\sqrt{1-x^2}} dx} - x\frac{\int_{-1}^{1} x \cdot x^2 \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} x \cdot x \frac{1}{\sqrt{1-x^2}} dx} = x^2 - \frac{1}{2}$$

$$\langle T_2 | T_2 \rangle = \int_{-1}^{1} a_2^2 (x^2 - \frac{1}{2})^2 \frac{1}{\sqrt{1-x^2}} dx = a_2^2 \frac{\pi}{8} = \frac{\pi}{2}$$

so $a_2 = 2$, and $T_2 = 2x^2 - 1$.

$$\varphi_3 = x^3 - 1\frac{\int_{-1}^{1} 1 \cdot x^3 \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} 1 \cdot 1 \frac{1}{\sqrt{1-x^2}} dx} - x\frac{\int_{-1}^{1} x \cdot x^3 \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} x \cdot x \frac{1}{\sqrt{1-x^2}} dx} - (2x^2 - 1)\frac{\int_{-1}^{1} (2x^2-1) x^3 \frac{1}{\sqrt{1-x^2}} dx}{\int_{-1}^{1} (2x^2-1)^2 \frac{1}{\sqrt{1-x^2}} dx} = x^3 - \frac{3}{4}x$$

$$\langle T_3 | T_3 \rangle = \int_{-1}^{1} a_3^2 (x^3 - \frac{3}{4}x)^2 \frac{1}{\sqrt{1-x^2}} dx = a_3^2 \frac{\pi}{32} = \frac{\pi}{2}$$

so $a_3 = 4$, and $T_3 = 4x^3 - 3x$.

5.2.6 Note that

$$\int_{-1}^{1} x^{2n+1} \sqrt{1-x^2} dx = 0$$

because $x^{2n+1}\sqrt{1-x^2}$ is an odd function.

Let φ_n be the non-scaled function, and $U_n = a_n \varphi_n$, so $\langle U_n | U_n \rangle = \int_{-1}^{1} a_n^2 \varphi_n^2 \sqrt{1-x^2} dx$. Then

$$\varphi_0 = 1$$

$$\langle U_0 | U_0 \rangle = \int_{-1}^{1} a_0^2 \sqrt{1-x^2} dx = a_0^2 \frac{\pi}{2} = \frac{\pi}{2}$$

so $a_0 = 1$, and $U_0 = 1$.

$$\varphi_1 = x - 1\frac{\int_{-1}^{1} 1 \cdot x \sqrt{1-x^2} dx}{\int_{-1}^{1} 1 \cdot 1 \sqrt{1-x^2} dx} = x$$

$$\langle U_1 | U_1 \rangle = \int_{-1}^{1} a_1^2 x^2 \sqrt{1-x^2} dx = a_1^2 \frac{\pi}{8} = \frac{\pi}{2}$$

so $a_1 = 2$, and $U_1 = 2x$.

$$\varphi_2 = x^2 - 1\frac{\int_{-1}^{1} 1 \cdot x^2 \sqrt{1-x^2} dx}{\int_{-1}^{1} 1 \cdot 1 \sqrt{1-x^2} dx} - 2x\frac{\int_{-1}^{1} 2x \cdot x^2 \sqrt{1-x^2} dx}{\int_{-1}^{1} 2x \cdot 2x \sqrt{1-x^2} dx} = x^2 - \frac{1}{4}$$

$$\langle U_2 | U_2 \rangle = \int_{-1}^{1} a_2^2 (x^2 - \frac{1}{4})^2 \sqrt{1-x^2} dx = a_2^2 \frac{\pi}{32} = \frac{\pi}{2}$$

so $a_2 = 4$, and $U_2 = 4x^2 - 1$.

5.2.7

$$\psi_0 = 1$$

$$\varphi_0 = 1$$

$$\psi_1 = x - 1\frac{\int_0^{\infty} 1 \cdot x e^{-x^2} dx}{\int_0^{\infty} 1 \cdot 1 e^{-x^2} dx} = x - \frac{1}{\sqrt{\pi}}$$

$$\varphi_1 = x - \frac{1}{\sqrt{\pi}}$$

5.2.8

$$\mathbf{a_1'} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\mathbf{a_1} = \frac{\mathbf{a_1'}}{(\mathbf{a_1'} \cdot \mathbf{a_1'})^{1/2}} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\mathbf{a_2'} = \mathbf{c_2} - \mathbf{a_1}(\mathbf{a_1} \cdot \mathbf{c_2}) = \frac{1}{3} \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix}$$

$$\mathbf{a_2} = \frac{\mathbf{a_2'}}{(\mathbf{a_2'} \cdot \mathbf{a_2'})^{1/2}} = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix}$$

$$\mathbf{a_3'} = \mathbf{c_3} - \mathbf{a_1}(\mathbf{a_1} \cdot \mathbf{c_3}) - \mathbf{a_2}(\mathbf{a_2} \cdot \mathbf{c_3}) = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

$$\mathbf{a_3} = \frac{\mathbf{a_3'}}{(\mathbf{a_3'} \cdot \mathbf{a_3'})^{1/2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

5.3 Operators

5.3.1

$$\langle f|Ag\rangle = \langle A^\dagger f|g\rangle = \langle g|A^\dagger f\rangle^* = \langle (A^\dagger)^\dagger g|f\rangle^* = \langle f|(A^\dagger)^\dagger g\rangle$$

so

$$\langle f|(A - (A^\dagger)^\dagger)g\rangle = 0$$

for any f and g. If $A - (A^\dagger)^\dagger \neq 0$, which means there are some g such that $(A - (A^\dagger)^\dagger)g = \varphi \neq 0$, then let $f = \varphi$, and $\langle f|(A - (A^\dagger)^\dagger)g\rangle = \langle \varphi|\varphi\rangle > 0$, contradict. So $A - (A^\dagger)^\dagger$ must be zero, which means

$$(A^\dagger)^\dagger = A$$

5.3.2

$$\langle f|UVg\rangle = \langle U^\dagger f|Vg\rangle = \langle V^\dagger U^\dagger f|g\rangle$$

also

$$\langle f|UVg\rangle = \langle (UV)^\dagger f|g\rangle$$

so

$$\langle ((UV)^\dagger - V^\dagger U^\dagger)f|g\rangle = 0$$

for any f and g, so $(UV)^\dagger - V^\dagger U^\dagger$ must be zero, which means

$$(UV)^\dagger = V^\dagger U^\dagger$$

5.3.3 (a)

$$(A_1)_{ij} = \langle \varphi_i|A_1|\varphi_j\rangle = \langle x_i|\sum_{k=1}^{3} x_k(\frac{\partial}{\partial x_k})|x_j\rangle = \langle x_i|x_j\rangle = \delta_{ij}$$

$$(A_2)_{ij} = \langle \varphi_i|A_2|\varphi_j\rangle = \langle x_i|x_1(\frac{\partial}{\partial x_2}) - x_2(\frac{\partial}{\partial x_1})|x_j\rangle = \langle x_i|x_1\delta_{2j} - x_2\delta_{1j}\rangle = \delta_{i1}\delta_{2j} - \delta_{i2}\delta_{1j}$$

In matrix forms,

$$\mathrm{A}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathrm{A}_2 \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

(b)

$$\psi_i = \langle \varphi_i|\psi\rangle = \langle x_i|x_1 - 2x_2 + 3x_3\rangle = \delta_{i1} - 2\delta_{i2} + 3\delta_{i3}$$

In matrix form,

$$\boldsymbol{\psi} = \begin{pmatrix} 1 \\ -2 \\ 3 \end{pmatrix}$$

(c) From matrix equation,

$$\boldsymbol{\chi} = \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} 1 \\ -2 \\ 3 \end{pmatrix} = \begin{pmatrix} 3 \\ -1 \\ 3 \end{pmatrix}$$

which is $3x_1 - x_2 + 3x_3$.

By direct application,

$$\chi = (A_1 - A_2)\psi = \sum_{i=1}^{3} x_i(\frac{\partial}{\partial x_i})(x_1 - 2x_2 + 3x_3) - \left[x_1(\frac{\partial}{\partial x_2}) - x_2(\frac{\partial}{\partial x_1}) \right] (x_1 - 2x_2 + 3x_3)$$

$$= x_1 - 2x_2 + 3x_3 - (-2x_1 - x_2) = 3x_1 - x_2 + 3x_3$$

which is the same with the results from matrix multiplication.

5.3.4 (a)

$$AP_0 = x\frac{d}{dx}(\frac{1}{\sqrt{2}}) = 0$$

$$AP_1 = x\frac{d}{dx}(\sqrt{\frac{3}{2}}x) = \sqrt{\frac{3}{2}}x = P_1$$

$$AP_2 = x\frac{d}{dx}\left(\sqrt{\frac{5}{2}}(\frac{3}{2}x^2 - \frac{1}{2})\right) = \sqrt{\frac{5}{2}}3x^2 = 2P_2 + \sqrt{5}P_0$$

$$AP_3 = x\frac{d}{dx}\left(\sqrt{\frac{7}{2}}(\frac{5}{2}x^3 - \frac{3}{2}x)\right) = \sqrt{\frac{7}{2}}\frac{15}{2}x^3 - \sqrt{\frac{7}{2}}\frac{3}{2}x = 3P_3 + \sqrt{21}P_1$$

We can evaluate A_{ij} by $A_{ij} = \langle P_i | AP_j \rangle$, and $\langle P_i | P_j \rangle = \delta_{ij}$. In matrix form,

$$\mathrm{A} = \begin{pmatrix} 0 & 0 & \sqrt{5} & 0 \\ 0 & 1 & 0 & \sqrt{21} \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$$

(b)

$$x^3 = P_0 \int_{-1}^{1} \frac{1}{\sqrt{2}} x^3 dx + P_1 \int_{-1}^{1} \sqrt{\frac{3}{2}}x \cdot x^3 dx + P_2 \int_{-1}^{1} \sqrt{\frac{5}{2}}(\frac{3}{2}x^2 - \frac{1}{2}) \cdot x^3 dx + P_3 \int_{-1}^{1} \sqrt{\frac{7}{2}}(\frac{5}{2}x^3 - \frac{3}{2}x)x^3 dx$$

$$= \frac{\sqrt{6}}{5}P_1 + \frac{2\sqrt{14}}{35}P_3$$

(c)

$$\begin{pmatrix} 0 & 0 & \sqrt{5} & 0 \\ 0 & 1 & 0 & \sqrt{21} \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{\sqrt{6}}{5} \\ 0 \\ \frac{2\sqrt{14}}{35} \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{3\sqrt{6}}{5} \\ 0 \\ \frac{6\sqrt{14}}{35} \end{pmatrix}$$

which is

$$\frac{3\sqrt{6}}{5}(\sqrt{\frac{3}{2}}x) + \frac{6\sqrt{14}}{35}\sqrt{\frac{7}{2}}(\frac{5}{2}x^3 - \frac{3}{2}x) = 3x^3$$

which is the same as $Ax^3 = x\frac{d}{dx}(x^3) = 3x^3$.

5.4 Self-Adjoint Operators

5.4.1 (a)

$$\langle f|(A+A^\dagger)g\rangle = \langle (A+A^\dagger)^\dagger f|g\rangle = \langle (A^\dagger + A)f|g\rangle = \langle (A+A^\dagger)f|g\rangle$$

$$\langle f|i(A-A^\dagger)g\rangle = \langle -i(A-A^\dagger)^\dagger f|g\rangle = \langle -i(A^\dagger - A)f|g\rangle = \langle i(A-A^\dagger)f|g\rangle$$

(b) For every operator A,

$$A = \frac{1}{2}(A+A^\dagger) - \frac{i}{2}i(A-A^\dagger)$$

where both $A+A^\dagger$ and $i(A-A^\dagger)$ are Hermitian.

5.4.2 Let A, B be Hermitian.

If AB is Hermitian, then $\langle f|ABg\rangle = \langle ABf|g\rangle$, but also

$$\langle f|ABg\rangle = \langle Af|Bg\rangle = \langle BAf|g\rangle$$

so $\langle (AB-BA)f|g\rangle = 0$ for any f, g, which means $(AB-BA)$ must be zero, and therefore $AB = BA$,

If $AB = BA$, then

$$\langle f|ABg\rangle = \langle Af|Bg\rangle = \langle BAf|g\rangle = \langle ABf|g\rangle$$

so AB is Hermitian.

5.4.3 A, B are Hermitian because they are quantum mechanical operators. $C = -i(AB-BA)$, so

$$\langle f|Cg\rangle = \langle C^\dagger d|g\rangle = \langle i(B^\dagger A^\dagger - A^\dagger B^\dagger)f|g\rangle = \langle i(BA-AB)f|g\rangle = \langle -i(AB-BA)f|g\rangle = \langle Cf|g\rangle$$

so C is Hermitian.

5.4.4 $\mathcal{L}$ is Hermitian, so

$$\langle\psi|\mathcal{L}^2|\psi\rangle = \langle\psi|\mathcal{L}\mathcal{L}|\psi\rangle = \langle\mathcal{L}\psi|\mathcal{L}\psi\rangle \geq 0$$

by the definition of scalar product.

5.4.5 (a) In spherical polar coordinate, $\varphi_1 = C\sin\theta\cos\varphi$, $\varphi_2 = C\sin\theta\sin\varphi$, $\varphi_3 = C\cos\theta$. So

$$\langle\varphi_1|\varphi_1\rangle = \int_0^\pi \int_0^{2\pi} (|C|^2 \sin^2\theta\cos^2\varphi)\sin\theta\, d\theta\, d\varphi$$

$$= |C|^2 \int_0^\pi \sin^3\theta\, d\theta \int_0^{2\pi} \cos^2\varphi\, d\varphi = |C|^2 \frac{4\pi}{3} = 1$$

so

$$C = \sqrt{\frac{3}{4\pi}} e^{i\theta}$$

By symmetry this C also made φ_2 and φ_3 normalized.

$$\langle\varphi_1|\varphi_2\rangle = \int_0^\pi \int_0^{2\pi} |C|^2 \sin^2\theta\cos^2\varphi\sin\theta\, d\theta\, d\varphi$$

$$= |C|^2 \int_0^\pi \sin^3\theta\, d\theta \int_0^{2\pi} \sin\varphi\cos\varphi\, d\varphi = 0$$

By symmetry $\langle\varphi_2|\varphi_3\rangle$ and $\langle\varphi_3|\varphi_1\rangle$ are also zero.

(b) Let i, j, k be a cyclic permutation of x, y, z, then all the three operators have the form

$$L_i = -i(x_j \frac{\partial}{\partial x_k} - x_k \frac{\partial}{\partial x_j})$$

Note that $\frac{\partial}{\partial x_k}(\frac{1}{r}) = -\frac{x_k}{r^3}$, so

$$L_i \varphi_b = -i\left[x_j \frac{\partial}{\partial x_k}(\frac{Cx_b}{r}) - x_k \frac{\partial}{\partial x_j}(\frac{Cx_b}{r})\right]$$

$$= -iC\left[x_j \frac{\partial x_b}{\partial x_k}\frac{1}{r} - x_j x_b \frac{x_k}{r^3} - x_k \frac{\partial x_b}{\partial x_j}\frac{1}{r} + x_k x_b \frac{x_j}{r^3}\right]$$

$$= -i\frac{C}{r}\left[x_j\delta_{kb} - x_k\delta_{jb}\right] = -i\left[\varphi_j\delta_{kb} - \varphi_k\delta_{jb}\right]$$

so

$$\langle\varphi_a|L_i|\varphi_b\rangle = -i\left[\langle\varphi_a|\varphi_j\rangle\delta_{kb} - \langle\varphi_a|\varphi_k\rangle\delta_{jb}\right] = -i\left(\delta_{aj}\delta_{kb} - \delta_{ak}\delta_{jb}\right)$$

$$= \begin{cases} -i & \textit{when } a = j,\ b = k \\ i & \textit{when } a = k,\ b = j \end{cases}$$

The components of L_i are $(L_i)_{ab} = \langle\varphi_a|L_i|\varphi_b\rangle$, so in matrix form,

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad L_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad L_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

(c)

$$L_xL_y - L_yL_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = iL_z$$

(we can prove $[L_x, L_y] = iL_z$, $[L_y, L_z] = iL_x$, $[L_z, L_x] = iL_y$ together: Note that

$$\langle\varphi_a|L_i|\varphi_b\rangle = \begin{cases} -i & \textit{when } a = j,\ b = k \\ i & \textit{when } a = k,\ b = j \end{cases}$$

is equivalent with $(L_i)_{ab} = -i\varepsilon_{iab}$. Let i, j, k be a cyclic permutation of x, y, z, then

$$(L_iL_j)_{ab} = \sum_c (L_i)_{ac}(L_j)_{cb} = \sum_c -\varepsilon_{iac}\varepsilon_{jcb} = -\varepsilon_{iak}\varepsilon_{jkb} = \varepsilon_{iak}\varepsilon_{jbk} = \delta_{ij}\delta_{ab} - \delta_{ib}\delta_{aj} = -\delta_{ib}\delta_{aj}$$

by Exercise 2.1.9. So

$$(L_iL_j - L_jL_i)_{ab} = -\delta_{ib}\delta_{aj} + \delta_{jb}\delta_{ai} = \sum_l \varepsilon_{ijl}\varepsilon_{abl} = \varepsilon_{ijk}\varphi_{abk} = \varepsilon_{abk} = i(-i\varepsilon_{kab}) = i(L_k)_{ab}$$

which means $[L_i, L_j] = iL_k$)

5.5 Unitary Operators

5.5.1 (There are mistakes in the matrix U given in the text: U_{33} should be $\frac{-i}{\sqrt{2}}$ and U_{43} should be $\frac{i}{\sqrt{2}}$. It can be verified by checking $\chi_3 = U_{33}\chi_3' + U_{43}\chi_4'$. The author probably forget to take the complex conjugate of χ_3' when calculating $\langle\chi_3'|\chi_3\rangle = \int_0^\pi\int_0^{2\pi}\sin\theta\, d\theta d\varphi(\chi_3')^*\chi_3$, as well as $\langle\chi_4'|\chi_3\rangle$.)

(a)

$$f(\theta, \varphi) = \mathbf{c} = \begin{pmatrix} 3 \\ 2i \\ -1 \\ 0 \\ 1 \end{pmatrix}$$

$$\mathbf{c}' = \mathrm{U}\mathbf{c} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 2i \\ -1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{5}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \\ 1 \end{pmatrix}$$

$$\sum_i c_i'\chi_i' = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta(\frac{1}{\sqrt{2}}e^{i\varphi} + \frac{5}{\sqrt{2}}e^{-i\varphi}) + \sqrt{\frac{15}{32\pi}}\sin^2\theta(\frac{i}{\sqrt{2}}e^{2i\varphi} - \frac{i}{\sqrt{2}}e^{-2i\varphi}) + \chi_5'$$
$$= 3\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\varphi - 2i\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\varphi - \sqrt{\frac{15}{4\pi}}\sin^2\theta\sin\varphi\cos\varphi + \chi_5$$
$$= 3\chi_1 - 2i\chi_2 - \chi_3 + \chi_5 = \sum_i c_i\chi_i = f(\theta,\varphi)$$

(b)

$$\mathrm{U}^{-1}\mathrm{U} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

5.5.2 (a) The transformation is $x = z'$, $y = y'$, $z = -x'$. The new basis is defined as $\varphi_1' = x'$, $\varphi_2' = y'$, $\varphi_3' = z'$, so $\varphi_1 = \varphi_3'$, $\varphi_2 = \varphi_2'$, $\varphi_3 = -\varphi_1'$, which in matrix representation becomes

$$\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

(b) The transformation corresponds to rotating $\frac{\pi}{2}$ counterclockwise about y-axis, so the Euler angles are $\alpha = 0$, $\beta = \frac{\pi}{2}$, $\gamma = 0$. By Eq. 3.37,

$$S(\alpha,\beta,\gamma) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

which is the same as (a).

(c)

$$\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 \\ -3 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ -3 \\ 2 \end{pmatrix}$$

so $f' = -x' - 3y' + 2z' = z - 3y + 2x = f$, consistent.

5.5.3 $\varphi_1' = -\varphi_3$, $\varphi_2' = \varphi_2$, $\varphi_3' = \varphi_1$, so the inverse transformation matrix is

$$\mathrm{U}' = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\mathrm{U}'\mathrm{U} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

so the two matrix are matrix inverses of each other.

5.5.4 (The transformation matrix V given is not unitary. A possible unitary V is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix}$$

which will be used to solve the problem.)

(a)

$$\begin{pmatrix} i\sin\theta & \cos\theta & 0 \\ -\cos\theta & i\sin\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ -1 \\ -2 \end{pmatrix} = \begin{pmatrix} -\cos\theta + 3i\sin\theta \\ -3\cos\theta - i\sin\theta \\ -2 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix} \begin{pmatrix} -\cos\theta + 3i\sin\theta \\ -3\cos\theta - i\sin\theta \\ -2 \end{pmatrix} = \begin{pmatrix} -\cos\theta + 3i\sin\theta \\ -3\cos^2\theta - i\sin\theta(\cos\theta + 2) \\ -3\sin\theta\cos\theta + i(2\cos\theta - \sin^2\theta) \end{pmatrix}$$

so

$$f(x) = (-\cos\theta + 3i\sin\theta)\chi_1 + (-3\cos^2\theta - i\sin\theta(\cos\theta + 2))\chi_2 + (-3\sin\theta\cos\theta + i(2\cos\theta - \sin^2\theta))\chi_3$$

(b)

$$(UV) = \begin{pmatrix} i\sin\theta & \cos\theta & 0 \\ -\cos\theta & i\sin\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix} = \begin{pmatrix} i\sin\theta & \cos^2\theta & i\sin\theta\cos\theta \\ -\cos\theta & i\sin\theta\cos\theta & -\sin^2\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix}$$

$$\begin{pmatrix} i\sin\theta & \cos^2\theta & i\sin\theta\cos\theta \\ -\cos\theta & i\sin\theta\cos\theta & -\sin^2\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix} \begin{pmatrix} 3 \\ -1 \\ -2 \end{pmatrix} = \begin{pmatrix} -\cos^2\theta + i\sin\theta(3 - 2\cos\theta) \\ -3\cos\theta + 2\sin^2\theta - i\sin\theta\cos\theta \\ -\sin\theta + 2i\cos\theta \end{pmatrix}$$

$$(VU) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta \\ 0 & \sin\theta & -i\cos\theta \end{pmatrix} \begin{pmatrix} i\sin\theta & \cos\theta & 0 \\ -\cos\theta & i\sin\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} i\sin\theta & \cos\theta & 0 \\ -\cos^2\theta & i\sin\theta\cos\theta & i\sin\theta \\ -\sin\theta\cos\theta & i\sin^2\theta & -i\cos\theta \end{pmatrix}$$

$$\begin{pmatrix} i\sin\theta & \cos\theta & 0 \\ -\cos^2\theta & i\sin\theta\cos\theta & i\sin\theta \\ -\sin\theta\cos\theta & i\sin^2\theta & -i\cos\theta \end{pmatrix} \begin{pmatrix} 3 \\ -1 \\ -2 \end{pmatrix} = \begin{pmatrix} -\cos\theta + 3i\sin\theta \\ -3\cos^2\theta - i\sin\theta(\cos\theta + 2) \\ -3\sin\theta\cos\theta + i(2\cos\theta - \sin^2\theta) \end{pmatrix}$$

So only applying VU gives the same answer as (a), which is quite obvious because U is applied first.

5.5.5 (a) Let the normalized $\mathcal{P}_n = a_n P_n$ and $\mathcal{F}_n = b_n P_n$. Let the factors a_n and b_n be positive real numbers (every $a_n e^{i\theta}$ can also normalize the functions, as well as $b_n e^{i\theta}$)

$$\int_{-1}^{1} |a_0|^2 P_0^2\,dx = |a_0|^2 2 = 1, \quad a_0 = \frac{1}{\sqrt{2}}, \quad \mathcal{P}_0 = \frac{1}{\sqrt{2}}$$

$$\int_{-1}^{1} |a_1|^2 P_1^2\,dx = |a_1|^2 \frac{2}{3} = 1, \quad a_1 = \sqrt{\frac{3}{2}}, \quad \mathcal{P}_1 = \sqrt{\frac{3}{2}}x$$

$$\int_{-1}^{1} |a_2|^2 P_2^2\,dx = |a_2|^2 \frac{2}{5} = 1, \quad a_2 = \sqrt{\frac{5}{2}}, \quad \mathcal{P}_2 = \sqrt{\frac{5}{2}}(\frac{3}{2}x^2 - \frac{1}{2})$$

$$\int_{-1}^{1} |b_0|^2 F_0^2\,dx = |b_0|^2 \frac{2}{5} = 1, \quad b_0 = \sqrt{\frac{5}{2}}, \quad \mathcal{F}_1 = \sqrt{\frac{5}{2}}x^2$$

$$\int_{-1}^{1} |b_1|^2 F_1^2\,dx = |b_1|^2 \frac{2}{3} = 1, \quad b_1 = \sqrt{\frac{3}{2}}, \quad \mathcal{F}_1 = \sqrt{\frac{3}{2}}x$$

$$\int_{-1}^{1} |b_2|^2 F_2^2\,dx = |b_2|^2 8 = 1, \quad b_2 = \frac{1}{\sqrt{8}}, \quad \mathcal{F}_2 = \frac{1}{\sqrt{8}}(5x^2 - 3)$$

(b) $U_{ij} = \int_{-1}^{1} F_i^* P_j\,dx$. Note that except $U_{00}, U_{02}, U_{11}, U_{20}, U_{22}$, all the other U_{ij} vanish because $F_i^* P_j$ are odd functions for these i, j.

$$U_{00} = \int_{-1}^{1} \frac{\sqrt{5}}{2}x^2\,dx = \frac{\sqrt{5}}{3}$$

$$U_{02} = \int_{-1}^{1} \frac{5}{2}(\frac{3}{2}x^4 - \frac{1}{2}x^2)\,dx = \frac{2}{3}$$

$$U_{11} = \int_{-1}^{1} \frac{3}{2} x^2 \, dx = 1$$

$$U_{20} = \int_{-1}^{1} \frac{1}{4}(5x^2 - 3) \, dx = -\frac{2}{3}$$

$$U_{22} = \int_{-1}^{1} \frac{\sqrt{5}}{4}(\frac{15}{2}x^4 - 7x^2 + \frac{3}{2}) \, dx = \frac{\sqrt{5}}{3}$$

so

$$\mathrm{U} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ -\frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix}$$

(c)$V_{ij} = \int_{-1}^{1} P_i^* F_j \, dx$. Note that except $V_{00}, V_{02}, V_{11}, V_{20}, V_{22}$, all the other V_{ij} vanish because $P_i^* F_j$ are odd functions for these i, j.

$$V_{00} = \int_{-1}^{1} \frac{\sqrt{5}}{2} x^2 \, dx = \frac{\sqrt{5}}{3}$$

$$V_{02} = \int_{-1}^{1} \frac{1}{4}(5x^2 - 3) \, dx = -\frac{2}{3}$$

$$V_{11} = \int_{-1}^{1} \frac{3}{2} x^2 \, dx = 1$$

$$V_{20} = \int_{-1}^{1} \frac{5}{2}(\frac{3}{2}x^4 - \frac{1}{2}x^2) \, dx = \frac{2}{3}$$

$$V_{22} = \int_{-1}^{1} \frac{\sqrt{5}}{4}(\frac{15}{2}x^4 - 7x^2 + \frac{3}{2}) \, dx = \frac{\sqrt{5}}{3}$$

so

$$\mathrm{V} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & -\frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix}$$

(d)

$$\mathrm{U}^{-1} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & -\frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} = \mathrm{V}$$

$$\mathrm{V}^{-1} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ -\frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} = \mathrm{U}$$

$$\mathrm{UU}^{-1} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ -\frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & -\frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathrm{VV}^{-1} = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & -\frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ -\frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(e)

$$\mathbf{f}_P = \begin{pmatrix} \int_{-1}^{1} (\frac{1}{\sqrt{2}})(5x^2 - 3x + 1) \, dx \\ \int_{-1}^{1} (\sqrt{\frac{3}{2}} x)(5x^2 - 3x + 1) \, dx \\ \int_{-1}^{1} \sqrt{\frac{5}{2}} (\frac{3}{2}x^2 - \frac{1}{2})(5x^2 - 3x + 1) \, dx \end{pmatrix} = \begin{pmatrix} \frac{8\sqrt{2}}{3} \\ -\sqrt{6} \\ \frac{2\sqrt{10}}{3} \end{pmatrix}$$

$$\mathbf{f}_F = \begin{pmatrix} \int_{-1}^{1}(\sqrt{\frac{5}{2}}x^2)(5x^2-3x+1)\,dx \\ \int_{-1}^{1}(\sqrt{\frac{3}{2}}x)(5x^2-3x+1)\,dx \\ \int_{-1}^{1}\frac{1}{\sqrt{8}}(5x^2-3)(5x^2-3x+1)\,dx \end{pmatrix} = \begin{pmatrix} \frac{4\sqrt{10}}{3} \\ -\sqrt{6} \\ -\frac{2\sqrt{2}}{3} \end{pmatrix}$$

$$\mathrm{U}\mathbf{f}_P = \begin{pmatrix} \frac{\sqrt{5}}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ -\frac{2}{3} & 0 & \frac{\sqrt{5}}{3} \end{pmatrix} \begin{pmatrix} \frac{8\sqrt{2}}{3} \\ -\sqrt{6} \\ \frac{2\sqrt{10}}{3} \end{pmatrix} = \begin{pmatrix} \frac{4\sqrt{10}}{3} \\ -\sqrt{6} \\ -\frac{2\sqrt{2}}{3} \end{pmatrix} = \mathbf{f}_F$$

5.6 Transformations of Operators

5.6.1 (a)

$$S_x = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & \frac{-i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} S_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{-1}{2} \end{pmatrix}$$

(b)

$$\langle \varphi_1' | \varphi_2' \rangle = \langle C(\alpha+\beta) | C(\alpha-\beta) \rangle = |C|^2(\langle\alpha|\alpha\rangle - \langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle - \langle\beta|\beta\rangle) = |C|^2(1-1) = 0$$

$$\langle \varphi_1' | \varphi_1' \rangle = \langle C(\alpha+\beta) | C(\alpha+\beta) \rangle = |C|^2(\langle\alpha|\alpha\rangle + \langle\alpha|\beta\rangle + \langle\beta|\alpha\rangle + \langle\beta|\beta\rangle) = |C|^2 2 = 1$$

so $C = \frac{1}{\sqrt{2}}$ can normalize φ_1' and φ_2'. The transformation matrix U is

$$\mathrm{U} = \begin{pmatrix} \langle \varphi_1' | \varphi_1 \rangle & \langle \varphi_1' | \varphi_2 \rangle \\ \langle \varphi_2' | \varphi_1 \rangle & \langle \varphi_2' | \varphi_2 \rangle \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$$

(c)

$$S_x' = \mathrm{U}S_x\mathrm{U}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{-1}{2} \end{pmatrix}$$

$$S_y' = \mathrm{U}S_y\mathrm{U}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{-i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 & \frac{i}{2} \\ \frac{-i}{2} & 0 \end{pmatrix}$$

$$S_z' = \mathrm{U}S_z\mathrm{U}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{-1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$$

5.6.2 (a) Note that $y\frac{\partial}{\partial z}(e^{-r^2}) - z\frac{\partial}{\partial y}(e^{-r^2}) = e^{-r^2}(-2r)(y\frac{z}{r} - z\frac{y}{r}) = 0$, so

$$L_x\varphi_1 = 0$$

$$L_x\varphi_2 = -iC(-ze^{-r^2}) = i\varphi_3$$

$$L_x\varphi_3 = -iC(ye^{-r^2}) = -i\varphi_2$$

so in matrix form,

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

(b)

$$L_x' = \mathrm{U}L_x\mathrm{U}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(c) φ_i' is the i^{th} column of U^{-1} in φ_i basis, so

$$\varphi_1' = Cxe^{-r^2} \quad \varphi_2' = C\frac{y+iz}{\sqrt{2}}e^{-r^2} \quad \varphi_3' = C\frac{y-iz}{\sqrt{2}}e^{-r^2}$$

$L_x\varphi_i'$ is the i^{th} column of L_x' in φ_i' basis, so

$$L_x\varphi_1' = 0 \quad L_x\varphi_2' = \varphi_2' = C\frac{y+iz}{\sqrt{2}}e^{-r^2} \quad L_x\varphi_3' = -\varphi_3' = -C\frac{y-iz}{\sqrt{2}}e^{-r^2}$$

5.6.3 Definition:

$$\varphi_1 = T_{11}\chi_1$$

$$\varphi_2 = T_{12}\chi_1 + T_{22}\chi_2$$

$$\varphi_3 = T_{13}\chi_1 + T_{23}\chi_2 + T_{33}\chi_3$$

$$\mathrm{T} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ 0 & T_{22} & T_{23} \\ 0 & 0 & T_{33} \end{pmatrix}$$

Let ψ_i be the orthogonalized but yet normalized functions, so

$$\psi_1 = \chi_1$$

$$\psi_2 = \chi_2 - \psi_1\frac{\langle\psi_1|\chi_2\rangle}{\langle\psi_1|\psi_1\rangle}$$

$$\psi_3 = \chi_3 - \psi_2\frac{\langle\psi_2|\chi_3\rangle}{\langle\psi_2|\psi_2\rangle} - \psi_1\frac{\langle\psi_1|\chi_3\rangle}{\langle\psi_1|\psi_1\rangle}$$

By comparing the coefficients of χ_n in φ_n and ψ_n, we have

$$\varphi_n = T_{nn}\psi_n$$

Let

$$S_{ij} = \langle\chi_i|\chi_j\rangle$$

$$\mathrm{S} = \begin{pmatrix} \langle\chi_1|\chi_1\rangle & \langle\chi_1|\chi_2\rangle & \langle\chi_1|\chi_3\rangle \\ \langle\chi_2|\chi_1\rangle & \langle\chi_2|\chi_2\rangle & \langle\chi_2|\chi_3\rangle \\ \langle\chi_3|\chi_1\rangle & \langle\chi_3|\chi_2\rangle & \langle\chi_3|\chi_3\rangle \end{pmatrix}$$

$$D_1 = \langle\chi_1|\chi_1\rangle$$

$$D_2 = \begin{vmatrix} \langle\chi_1|\chi_1\rangle & \langle\chi_1|\chi_2\rangle \\ \langle\chi_2|\chi_1\rangle & \langle\chi_2|\chi_2\rangle \end{vmatrix}$$

$$D_3 = \begin{vmatrix} \langle\chi_1|\chi_1\rangle & \langle\chi_1|\chi_2\rangle & \langle\chi_1|\chi_3\rangle \\ \langle\chi_2|\chi_1\rangle & \langle\chi_2|\chi_2\rangle & \langle\chi_2|\chi_3\rangle \\ \langle\chi_3|\chi_1\rangle & \langle\chi_3|\chi_2\rangle & \langle\chi_3|\chi_3\rangle \end{vmatrix}$$

Note that $S_{ij}^* = \langle\chi_j|\chi_1\rangle$, $D_n^* = D_n$. In this problem when $|A|^2 = k$, let $A = \sqrt{k}$, without the phase factor.

From Eq. 5.79 we have

$$\mathrm{T}^\dagger\mathrm{S}\mathrm{T} = \mathrm{I}$$

note that from the derivation, the equation will hold for any dimension, so

$$T_{11}^*\langle\chi_1|\chi_1\rangle T_{11} = 1$$

$$T_{11} = \frac{1}{\sqrt{D_1}}$$

$$\begin{pmatrix} T_{11}^* & 0 \\ T_{12}^* & T_{22}^* \end{pmatrix} \begin{pmatrix} \langle\chi_1|\chi_1\rangle & \langle\chi_1|\chi_2\rangle \\ \langle\chi_2|\chi_1\rangle & \langle\chi_2|\chi_2\rangle \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Take the determinant of both sides:

$$T_{11}^* T_{22}^* D_2 T_{11} T_{22} = 1$$

$$|T_{22}|^2 = \frac{1}{|T_{11}|^2 D_2} = \frac{D_1}{D_2}, \quad T_{22} = \sqrt{\frac{D_1}{D_2}}$$

$$\begin{pmatrix} T_{11}^* & 0 & 0 \\ T_{12}^* & T_{22}^* & 0 \\ T_{13}^* & T_{23}^* & T_{33}^* \end{pmatrix} \begin{pmatrix} \langle\chi_1|\chi_1\rangle & \langle\chi_1|\chi_2\rangle & \langle\chi_1|\chi_3\rangle \\ \langle\chi_2|\chi_1\rangle & \langle\chi_2|\chi_2\rangle & \langle\chi_2|\chi_3\rangle \\ \langle\chi_3|\chi_1\rangle & \langle\chi_3|\chi_2\rangle & \langle\chi_3|\chi_3\rangle \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ 0 & T_{22} & T_{23} \\ 0 & 0 & T_{33} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T_{11}^* T_{22}^* T_{33}^* D_2 T_{11} T_{22} T_{33} = 1$$

$$|T_{33}|^2 = \frac{1}{|T_{22}|^2 |T_{11}|^2 D_3} = \frac{D_2}{D_3}, \quad T_{33} = \sqrt{\frac{D_2}{D_3}}$$

$$\psi_1 = \chi_1$$

$$\varphi_1 = T_{11}\chi_1 = \frac{\chi_1}{\sqrt{D_1}}$$

$$\psi_2 = \chi_2 - \psi_1 \frac{\langle\psi_1|\chi_2\rangle}{\langle\psi_1|\psi_1\rangle} = \chi_2 - \chi_1 \frac{S_{12}}{S_{11}}$$

$$\varphi_2 = T_{22}\psi_2 = \sqrt{\frac{D_1}{D_2}}(\chi_1 \frac{-S_{12}}{S_{11}} + \chi_2) = \chi_1 \frac{-S_{12}}{\sqrt{D_1 D_2}} + \chi_2 \sqrt{\frac{D_1}{D_2}}$$

$$\psi_3 = \chi_3 - \psi_2 \frac{\langle\psi_2|\chi_3\rangle}{\langle\psi_2|\psi_2\rangle} - \psi_1 \frac{\langle\psi_1|\chi_3\rangle}{\langle\psi_1|\psi_1\rangle}$$

$$= \chi_3 - (\chi_2 - \chi_1 \frac{S_{12}}{S_{11}}) \frac{S_{23} - S_{13}\frac{S_{21}}{S_{11}}}{S_{22} - \frac{S_{12}S_{21}}{S_{11}}} - \chi_1 \frac{S_{13}}{S_{11}}$$

$$= \chi_3 + \chi_2 \frac{S_{13}S_{21} - S_{11}S_{23}}{S_{11}S_{22} - S_{12}S_{21}} + \chi_1 \frac{S_{11}S_{12}S_{13} - S_{12}S_{21}S_{13} - S_{11}S_{22}S_{13} + S_{12}S_{21}S_{13}}{(S_{11}S_{22} - S_{12}S_{21})S_{11}}$$

$$= \chi_3 + \chi_2 \frac{S_{13}S_{21} - S_{11}S_{23}}{D_2} + \chi_1 \frac{S_{11}S_{12}S_{13} - S_{12}S_{21}S_{13} - S_{11}S_{22}S_{13} + S_{12}S_{21}S_{13}}{D_2 D_1}$$

$$\varphi_3 = T_{33}\psi_3 = \chi_3 \sqrt{\frac{D_2}{D_3}} + \chi_2 \frac{S_{13}S_{21} - S_{11}S_{23}}{\sqrt{D_2 D_3}} + \chi_1 \frac{S_{11}S_{12}S_{13} - S_{12}S_{21}S_{13} - S_{11}S_{22}S_{13} + S_{12}S_{21}S_{13}}{D_1 \sqrt{D_2 D_3}}$$

so

$$\mathrm{T} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ 0 & T_{22} & T_{23} \\ 0 & 0 & T_{33} \end{pmatrix}$$

$$T_{11} = \frac{1}{\sqrt{D_1}}$$

$$T_{12} = \frac{-S_{12}}{\sqrt{D_1 D_2}}$$

$$T_{22} = \sqrt{\frac{D_1}{D_2}}$$

$$T_{13} = \frac{S_{11}S_{12}S_{13} - S_{12}S_{21}S_{13} - S_{11}S_{22}S_{13} + S_{12}S_{21}S_{13}}{D_1 \sqrt{D_2 D_3}}$$

$$T_{23} = \frac{S_{13}S_{21} - S_{11}S_{23}}{\sqrt{D_2 D_3}}$$

$$T_{33} = \sqrt{\frac{D_2}{D_3}}$$

5.7 Invariants

5.7.1 In matrix representation,

$$\begin{aligned}
\mathrm{XP} - \mathrm{PX} &= i\mathrm{I} \\
\mathrm{UXPU}^{-1} - \mathrm{UPXU}^{-1} &= i\mathrm{UIU}^{-1} = i\mathrm{I} \\
\mathrm{UXU}^{-1}\mathrm{UPU}^{-1} - \mathrm{UPU}^{-1}\mathrm{UXU}^{-1} &= i\mathrm{I} \\
\mathrm{X}'\mathrm{P}' - \mathrm{P}'\mathrm{X}' &= i\mathrm{I}
\end{aligned}$$

so $[x, p] = i$ is invariant under unitary transformation.

5.7.2

$$\boldsymbol{\sigma}_1' = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \sin 2\theta & \cos 2\theta \\ \cos 2\theta & -\sin 2\theta \end{pmatrix}$$

$$\boldsymbol{\sigma}_2' = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\boldsymbol{\sigma}_3' = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ -\sin 2\theta & -\cos 2\theta \end{pmatrix}$$

$$\boldsymbol{\sigma}_1'\boldsymbol{\sigma}_2' - \boldsymbol{\sigma}_2'\boldsymbol{\sigma}_1' = \begin{pmatrix} i\cos 2\theta & -i\sin 2\theta \\ -i\sin 2\theta & -i\cos 2\theta \end{pmatrix} - \begin{pmatrix} -i\cos 2\theta & i\sin 2\theta \\ i\sin 2\theta & i\cos 2\theta \end{pmatrix} = \begin{pmatrix} 2i\cos 2\theta & -2i\sin 2\theta \\ -2i\sin 2\theta & -2i\cos 2\theta \end{pmatrix} = 2i\boldsymbol{\sigma}_3'$$

so $[\boldsymbol{\sigma}_1', \boldsymbol{\sigma}_2'] = 2i\boldsymbol{\sigma}_3'$ is still valid under transformation.

5.7.3 (a) From Exercise 5.6.2(a),

$$\begin{aligned}
L_x\varphi_1 &= 0 \\
L_x\varphi_2 &= -iC(-ze^{-r^2}) = i\varphi_3 \\
L_x\varphi_3 &= -iC(ye^{-r^2}) = -i\varphi_2
\end{aligned}$$

so in matrix form,

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

(b)

$$L_x\left[(x+iy)e^{-r^2}\right] = L_x\frac{\varphi_1 + i\varphi_2}{C} = \frac{i(i\varphi_3)}{C} = -\frac{\varphi_3}{C} = -ze^{-r^2}$$

(c) In matrix form, the above equation becomes

$$\begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$

after transformation,

$$\begin{pmatrix} 0 \\ \frac{i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

where the transformed L_x has been obtained in Exercise 5.6.2(b).

(d) From Exercise 5.6.2(c),

$$\varphi_1' = Cxe^{-r^2} \qquad \varphi_2' = C\frac{y+iz}{\sqrt{2}}e^{-r^2} \qquad \varphi_3' = C\frac{y-iz}{\sqrt{2}}e^{-r^2}$$

(e)

$$\varphi_2'\frac{i}{\sqrt{2}} + \varphi_3'\frac{-i}{\sqrt{2}} = -Cze^{-r^2}$$

$$\varphi_1' + \varphi_2' \frac{i}{\sqrt{2}} + \varphi_3' \frac{i}{\sqrt{2}} = C(x+iy)e^{-r^2}$$

$$L_x \varphi_1' = L_x(Cxe^{-r^2}) = 0$$

$$L_x \varphi_2' = L_x(C\frac{y+iz}{\sqrt{2}}e^{-r^2}) = C\frac{y+iz}{\sqrt{2}}e^{-r^2} = \varphi_2'$$

$$L_x \varphi_3' = L_x(C\frac{y-iz}{\sqrt{2}}e^{-r^2}) = -C\frac{y-iz}{\sqrt{2}}e^{-r^2} = -\varphi_3'$$

so the vectors and operators transform correctly by U.