Physics 741 – Graduate Quantum Mechanics 1

Solutions to Chapter 3

3.1 [5] Prove Schwartz's inequality, $(\phi,\psi)(\psi,\phi) \le (\phi,\phi)(\psi,\psi)$. You may prove it however you want; however, here is one way to prove it. Expand out the inner product of $a\phi + b\psi$ with itself, which must be positive, where *a* and *b* are arbitrary *complex* numbers. Then substitute in $a = (\phi,\psi)$ and $b = -(\phi,\phi)$. Simplify, and you should have the desired result.

We take the suggestion given, hoping it will not lead us astray. We note that *b* is real, so $b^* = b = -(\phi,\phi)$, while *a* is not, so $a^* = (\phi,\psi)^* = (\psi,\phi)$.

$$\begin{aligned} 0 &\le (a\phi + b\psi, a\phi + b\psi) = a^* a(\phi,\phi) + a^* b(\phi,\psi) + b^* a(\psi,\phi) + b^* b(\psi,\psi) \\ &= (\psi,\phi)(\phi,\psi)(\phi,\phi) - (\psi,\phi)(\phi,\phi)(\phi,\psi) - (\phi,\phi)(\phi,\psi)(\psi,\phi) + (\phi,\phi)(\phi,\phi)(\psi,\psi) \\ &= -(\phi,\phi)(\phi,\psi)(\psi,\phi) + (\phi,\phi)(\phi,\phi)(\psi,\psi). \end{aligned}$$

We now rearrange this and divide by (ϕ,ϕ) to give $(\phi,\psi)(\psi,\phi) \le (\phi,\phi)(\psi,\psi)$, the desired relationship. The only detail that might be unclear is that in the ultimate step, we divided by (ϕ,ϕ). This is valid, provided $(\phi,\phi) > 0$, which is guaranteed for $\phi \ne 0$. Of course, if $\phi = 0$, then both sides of Schwartz's inequality are zero, and the result is trivially true.

3.2 [15] Our goal in this problem is to develop an orthonormal basis for polynomial functions on the interval $[-1,1]$, with inner product defined by $\langle f | g \rangle = \int_{-1}^{1} f^*(x) g(x)\,dx$. Consider the basis function $|\phi_n\rangle$, for $n = 0,1,2,\ldots$, defined by $\phi_n(x) = x^n$.

(a) [7] Find the inner product $\langle \phi_n | \phi_m \rangle$ for arbitrary *n*, *m*, and then use (3.25) to produce a set of orthogonal states $|\phi_n'\rangle$ for *n* up to 4.

The inner product is simply

$$\langle \phi_n | \phi_m \rangle = \int_{-1}^{1} x^n x^m dx = \left.\frac{x^{n+m+1}}{n+m+1}\right|_{-1}^{1} = \frac{1-(-1)^{n+m+1}}{n+m+1} = \begin{cases} 2/(n+m+1) & \text{if } n+m \text{ even,} \\ 0 & \text{if } n+m \text{ odd.} \end{cases}$$

We now simply produce a set of orthonormal states following the prescription given in (3.25):

$$|\phi_0'\rangle = |\phi_0\rangle,$$

$$|\phi_1'\rangle = |\phi_1\rangle - |\phi_0'\rangle\langle\phi_0'|\phi_1\rangle / \langle\phi_0'|\phi_0'\rangle = |\phi_1\rangle,$$

$$|\phi_2'\rangle = |\phi_2\rangle - |\phi_0'\rangle\langle\phi_0'|\phi_2\rangle / \langle\phi_0'|\phi_0'\rangle = |\phi_2\rangle - |\phi_0\rangle\langle\phi_0|\phi_2\rangle / \langle\phi_0|\phi_0\rangle = |\phi_2\rangle - |\phi_0\rangle\left(\tfrac{2}{3}/\tfrac{2}{1}\right) = |\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle$$

$$|\phi_3'\rangle = |\phi_2\rangle - |\phi_1'\rangle\langle\phi_1'|\phi_3\rangle / \langle\phi_1'|\phi_1'\rangle = |\phi_3\rangle - |\phi_1\rangle\langle\phi_1|\phi_3\rangle / \langle\phi_1|\phi_1\rangle = |\phi_3\rangle - |\phi_1\rangle\left(\tfrac{2}{5}/\tfrac{2}{3}\right) = |\phi_3\rangle - \tfrac{3}{5}|\phi_1\rangle,$$

$$\begin{aligned}
|\phi_4'\rangle &= |\phi_4\rangle - |\phi_0'\rangle\langle\phi_0'|\phi_4\rangle/\langle\phi_0'|\phi_0'\rangle - |\phi_2'\rangle\langle\phi_2'|\phi_4\rangle/\langle\phi_2'|\phi_2'\rangle \\
&= |\phi_4\rangle - |\phi_0\rangle\frac{\langle\phi_0|\phi_4\rangle}{\langle\phi_0|\phi_0\rangle} - \left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right)\frac{\left(\langle\phi_2| - \tfrac{1}{3}\langle\phi_0|\right)|\phi_4\rangle}{\left(\langle\phi_2| - \tfrac{1}{3}\langle\phi_0|\right)\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right)} \\
&= |\phi_4\rangle - |\phi_0\rangle\frac{\frac{2}{5}}{\frac{2}{1}} - \left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right)\frac{\frac{2}{7} - \frac{1}{3}\cdot\frac{2}{5}}{\frac{2}{5} - 2\cdot\frac{1}{3}\cdot\frac{2}{3} + \frac{1}{9}\cdot\frac{2}{1}} = |\phi_4\rangle - \tfrac{1}{5}|\phi_0\rangle - \tfrac{90-42}{126-140+70}\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right) \\
&= |\phi_4\rangle - \tfrac{1}{5}|\phi_0\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{2}{7}|\phi_0\rangle = |\phi_4\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{3}{35}|\phi_0\rangle .
\end{aligned}$$

(b) [6] Now produce a set of orthonormal states $|\phi_n''\rangle$ using (3.26) for *n* up to 4.

This is now straightforward. We find

$$\begin{aligned}
|\phi_0''\rangle &= \frac{1}{\sqrt{\langle\phi_0'|\phi_0'\rangle}}|\phi_0'\rangle = \frac{1}{\sqrt{\langle\phi_0|\phi_0\rangle}}|\phi_0\rangle = \frac{1}{\sqrt{\frac{2}{1}}}|\phi_0\rangle = \sqrt{\tfrac{1}{2}}|\phi_0\rangle , \\
|\phi_1''\rangle &= \frac{1}{\sqrt{\langle\phi_1|\phi_1\rangle}}|\phi_1\rangle = \frac{1}{\sqrt{\frac{2}{3}}}|\phi_1\rangle = \sqrt{\tfrac{3}{2}}|\phi_1\rangle \\
|\phi_2''\rangle &= \frac{1}{\sqrt{\left(\langle\phi_2| - \tfrac{1}{3}\langle\phi_0|\right)\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right)}}\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right) = \frac{1}{\sqrt{\frac{2}{5} - 2\cdot\frac{1}{3}\cdot\frac{2}{3} + \frac{1}{9}\cdot\frac{2}{1}}}\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right) \\
&= \sqrt{\tfrac{45}{8}}\left(|\phi_2\rangle - \tfrac{1}{3}|\phi_0\rangle\right) = \tfrac{1}{2}\sqrt{\tfrac{5}{2}}\left(3|\phi_2\rangle - |\phi_0\rangle\right), \\
|\phi_3''\rangle &= \frac{1}{\sqrt{\left(\langle\phi_3| - \tfrac{3}{5}\langle\phi_1|\right)\left(|\phi_3\rangle - \tfrac{3}{5}|\phi_1\rangle\right)}}\left(|\phi_3\rangle - \tfrac{3}{5}|\phi_1\rangle\right) = \frac{1}{\sqrt{\frac{2}{7} - 2\cdot\frac{3}{5}\cdot\frac{2}{5} + \frac{9}{25}\cdot\frac{2}{3}}}\left(|\phi_3\rangle - \tfrac{3}{5}|\phi_1\rangle\right) \\
&= \sqrt{\tfrac{175}{8}}\left(|\phi_3\rangle - \tfrac{3}{5}|\phi_1\rangle\right) = \tfrac{1}{2}\sqrt{\tfrac{7}{2}}\left(5|\phi_3\rangle - 3|\phi_1\rangle\right), \\
|\phi_4''\rangle &= \frac{1}{\sqrt{\left(\langle\phi_4| - \tfrac{6}{7}\langle\phi_2| + \tfrac{3}{35}\langle\phi_0|\right)\left(|\phi_4\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{3}{35}|\phi_0\rangle\right)}}\left(|\phi_4\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{3}{35}|\phi_0\rangle\right) \\
&= \frac{1}{\sqrt{\frac{2}{9} - 2\cdot\frac{6}{7}\cdot\frac{2}{7} + 2\cdot\frac{3}{35}\cdot\frac{2}{5} + \frac{36}{49}\cdot\frac{2}{5} - 2\cdot\frac{6}{7}\cdot\frac{3}{35}\cdot\frac{2}{3} + \frac{9}{1225}\cdot\frac{2}{1}}}\left(|\phi_4\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{3}{35}|\phi_0\rangle\right) \\
&= \sqrt{\tfrac{11025}{128}}\left(|\phi_4\rangle - \tfrac{6}{7}|\phi_2\rangle + \tfrac{3}{35}|\phi_0\rangle\right) = \tfrac{3}{8\sqrt{2}}\left(35|\phi_4\rangle - 30|\phi_2\rangle + 3|\phi_0\rangle\right).
\end{aligned}$$

(c) [2] Compare the resulting polynomials with Legendre polynomials. How are they related?

The Legendre polynomials can be found in a variety of sources, such as Wikipedia. The first five are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \tfrac{1}{2}\left(3x^2 - 1\right), \quad P_3(x) = \tfrac{1}{2}\left(5x^3 - 3x\right), \quad P_4(x) = \tfrac{1}{8}\left(35x^4 - 30x^2 + 3\right).$$

Comparing with the expressions above, we see that

$$\phi_0''(x) = \sqrt{\tfrac{1}{2}} P_0(x), \quad \phi_1''(x) = \sqrt{\tfrac{3}{2}} P_1(x), \quad \phi_2''(x) = \sqrt{\tfrac{5}{2}} P_0(x), \quad \phi_3''(x) = \sqrt{\tfrac{7}{2}} P_3(x),$$
$$\phi_4''(x) = \tfrac{3}{\sqrt{2}} P_4(x).$$

The pattern is clear: $\phi_n''(x) = \sqrt{\tfrac{2n+1}{2}} P_n(x)$.