

Physics 741 – Graduate Quantum Mechanics 1
Solutions to Chapter 3

1. [5] Prove Schwartz's inequality, $(\phi, \psi)(\psi, \phi) \leq (\phi, \phi)(\psi, \psi)$. 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 $a^* = (\phi, \psi)^* = (\psi, \phi)$.

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

We now rearrange this and divide by (ϕ, ϕ) to give $(\phi, \psi)(\psi, \phi) \leq (\phi, \phi)(\psi, \psi)$, 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 $\phi \neq 0$. Of course, if $\phi = 0$, then both sides of Schwartz's inequality are zero, and the result is trivially true.

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 $n = 0, 1, 2, \dots$, 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

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

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

$$\begin{aligned}
|\phi'_0\rangle &= |\phi_0\rangle, \\
|\phi'_1\rangle &= |\phi_1\rangle - |\phi'_0\rangle\langle\phi'_0|\phi_1\rangle/\langle\phi'_0|\phi'_0\rangle = |\phi_1\rangle, \\
|\phi'_2\rangle &= |\phi_2\rangle - |\phi'_0\rangle\langle\phi'_0|\phi_2\rangle/\langle\phi'_0|\phi'_0\rangle = |\phi_2\rangle - |\phi_0\rangle\langle\phi_0|\phi_2\rangle/\langle\phi_0|\phi_0\rangle = |\phi_2\rangle - |\phi_0\rangle(\frac{2}{3}/\frac{2}{1}) = |\phi_2\rangle - \frac{1}{3}|\phi_0\rangle \\
|\phi'_3\rangle &= |\phi_2\rangle - |\phi'_1\rangle\langle\phi'_1|\phi_3\rangle/\langle\phi'_1|\phi'_1\rangle = |\phi_3\rangle - |\phi_1\rangle\langle\phi_1|\phi_3\rangle/\langle\phi_1|\phi_1\rangle = |\phi_3\rangle - |\phi_1\rangle(\frac{2}{5}/\frac{2}{3}) = |\phi_3\rangle - \frac{3}{5}|\phi_1\rangle, \\
|\phi'_4\rangle &= |\phi_4\rangle - |\phi'_0\rangle\langle\phi'_0|\phi_4\rangle/\langle\phi'_0|\phi'_0\rangle - |\phi'_2\rangle\langle\phi'_2|\phi_4\rangle/\langle\phi'_2|\phi'_2\rangle \\
&= |\phi_4\rangle - |\phi_0\rangle\frac{\langle\phi_0|\phi_4\rangle}{\langle\phi_0|\phi_0\rangle} - (|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle)\frac{(\langle\phi_2|-\frac{1}{3}\langle\phi_0|)|\phi_4\rangle}{(\langle\phi_2|-\frac{1}{3}\langle\phi_0|)(|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle)} \\
&= |\phi_4\rangle - |\phi_0\rangle\frac{\frac{2}{5}}{\frac{2}{1}} - (|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle)\frac{\frac{2}{7} - \frac{1}{3}\cdot\frac{2}{5}}{\frac{2}{5} - 2\cdot\frac{1}{3}\cdot\frac{2}{3} + \frac{1}{9}\cdot\frac{2}{1}} = |\phi_4\rangle - \frac{1}{5}|\phi_0\rangle - \frac{90-42}{126-140+70}(|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle) \\
&= |\phi_4\rangle - \frac{1}{5}|\phi_0\rangle - \frac{6}{7}|\phi_2\rangle + \frac{2}{7}|\phi_0\rangle = |\phi_4\rangle - \frac{6}{7}|\phi_2\rangle + \frac{3}{35}|\phi_0\rangle.
\end{aligned}$$

(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^n\rangle &= \frac{|\phi'_0\rangle}{\sqrt{\langle\phi'_0|\phi'_0\rangle}} = \frac{|\phi_0\rangle}{\sqrt{\langle\phi_0|\phi_0\rangle}} = \frac{1}{\sqrt{\frac{2}{1}}}|\phi_0\rangle = \sqrt{\frac{1}{2}}|\phi_0\rangle, \\
|\phi_1^n\rangle &= \frac{|\phi_1\rangle}{\sqrt{\langle\phi_1|\phi_1\rangle}} = \frac{1}{\sqrt{\frac{2}{3}}}|\phi_1\rangle = \sqrt{\frac{3}{2}}|\phi_1\rangle \\
|\phi_2^n\rangle &= \frac{|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle}{\sqrt{(\langle\phi_2|-\frac{1}{3}\langle\phi_0|)(|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle)}} = \frac{|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle}{\sqrt{\frac{2}{5} - 2\cdot\frac{1}{3}\cdot\frac{2}{3} + \frac{1}{9}\cdot\frac{2}{1}}} = \sqrt{\frac{45}{8}}(|\phi_2\rangle - \frac{1}{3}|\phi_0\rangle) \\
&= \frac{1}{2}\sqrt{\frac{5}{2}}(3|\phi_2\rangle - |\phi_0\rangle), \\
|\phi_3^n\rangle &= \frac{|\phi_3\rangle - \frac{3}{5}|\phi_1\rangle}{\sqrt{(\langle\phi_3|-\frac{3}{5}\langle\phi_1|)(|\phi_3\rangle - \frac{3}{5}|\phi_1\rangle)}} = \frac{|\phi_3\rangle - \frac{3}{5}|\phi_1\rangle}{\sqrt{\frac{2}{7} - 2\cdot\frac{3}{5}\cdot\frac{2}{5} + \frac{9}{25}\cdot\frac{2}{3}}} = \sqrt{\frac{175}{8}}(|\phi_3\rangle - \frac{3}{5}|\phi_1\rangle) \\
&= \frac{1}{2}\sqrt{\frac{7}{2}}(5|\phi_3\rangle - 3|\phi_1\rangle), \\
|\phi_4^n\rangle &= \frac{|\phi_4\rangle - \frac{6}{7}|\phi_2\rangle + \frac{3}{35}|\phi_0\rangle}{\sqrt{(\langle\phi_4|-\frac{6}{7}\langle\phi_2|+\frac{3}{35}\langle\phi_0|)(|\phi_4\rangle - \frac{6}{7}|\phi_2\rangle + \frac{3}{35}|\phi_0\rangle)}} \\
&= \frac{|\phi_4\rangle - \frac{6}{7}|\phi_2\rangle + \frac{3}{35}|\phi_0\rangle}{\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}}} = \sqrt{\frac{11025}{128}}(|\phi_4\rangle - \frac{6}{7}|\phi_2\rangle + \frac{3}{35}|\phi_0\rangle) \\
&= \frac{3}{8\sqrt{2}}(35|\phi_4\rangle - 30|\phi_2\rangle + 3|\phi_0\rangle).
\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

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

Comparing with the expressions above, we see that

$$\phi_0''(x) = \sqrt{\frac{1}{2}}P_0(x), \quad \phi_1''(x) = \sqrt{\frac{3}{2}}P_1(x), \quad \phi_2''(x) = \sqrt{\frac{5}{2}}P_2(x), \quad \phi_3''(x) = \sqrt{\frac{7}{2}}P_3(x), \\ \phi_4''(x) = \frac{3}{\sqrt{2}}P_4(x).$$

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

3. [10] Prove the following identities about the operators A , B , and C :

(a) [4] Commutators of products:

$$[A, BC] = B[A, C] + [A, B]C \quad \text{and} \quad [AB, C] = A[B, C] + [A, C]B$$

You simply write out the right side explicitly in each case and then simplify it to give the left side.

$$B[A, C] + [A, B]C = BAC - BCA + ABC - BAC = ABC - BCA = [A, BC], \\ A[B, C] + [A, C]B = ABC - ACB + ACB - CAB = ABC - CAB = [AB, C].$$

(b) [4] The Jacobi identities:

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \quad \text{and} \\ [[A, B], C] + [[B, C], A] + [[C, A], B] = 0$$

You simply write everything out explicitly in each case, and you find everything cancels beautifully:

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = [A, BC - CB] + [B, CA - AC] + [C, AB - BA] \\ = ABC - BCA - ACB - CBA + BCA - CAB - BAC + ACB + CAB - ABC - CBA + BAC = 0, \\ [[A, B], C] + [[B, C], A] + [[C, A], B] = [AB - BA, C] + [BC - CB, A] + [CA - AC, B] \\ = ABC - CAB - BAC + CBA + BCA - ABC - CBA + ACB + CAB - BCA - ACB + BAC = 0.$$

(c) [2] Show that if A and B are Hermitian, then $i[A, B]$ is also Hermitian

$$\{i[A, B]\}^\dagger = \{iAB - iBA\}^\dagger = B^\dagger A^\dagger (-i) - A^\dagger B^\dagger (-i) = iAB - iBA = i[A, B]$$

4. [10] Define the angular momentum operators $\mathbf{L} = \mathbf{R} \times \mathbf{P}$, or in components

$$L_x = YP_z - ZP_y, \quad L_y = ZP_x - XP_z, \quad L_z = XP_y - YP_x$$

(a) [6] With the help of problem 3(a), work out the six commutators $[L_z, \mathbf{R}]$ and $[L_z, \mathbf{P}]$.

$$\begin{aligned} [L_z, X] &= [XP_y - YP_x, X] = X[P_y, X] + [X, X]P_y - Y[P_x, X] - [Y, X]P_x = -Y(-i\hbar) = i\hbar Y, \\ [L_z, Y] &= [XP_y - YP_x, Y] = X[P_y, Y] + [X, Y]P_y - Y[P_x, Y] - [Y, Y]P_x = X(-i\hbar) = -i\hbar X, \\ [L_z, Z] &= [XP_y - YP_x, Z] = X[P_y, Z] + [X, Z]P_y - Y[P_x, Z] - [Y, Z]P_x = 0, \\ [L_z, P_x] &= [XP_y - YP_x, P_x] = X[P_y, P_x] + [X, P_x]P_y - Y[P_x, P_x] - [Y, P_x]P_x = (i\hbar)P_y = i\hbar P_y, \\ [L_z, P_y] &= [XP_y - YP_x, P_y] = X[P_y, P_y] + [X, P_y]P_y - Y[P_x, P_y] - [Y, P_y]P_x = -(i\hbar)P_x \\ &= -i\hbar P_x, \\ [L_z, P_z] &= [XP_y - YP_x, P_z] = X[P_y, P_z] + [X, P_z]P_y - Y[P_x, P_z] - [Y, P_z]P_x = 0. \end{aligned}$$

(b) [4] With the help of problems 3(a) and 4(a), work out the commutators $[L_z, L_x]$ and $[L_z, L_y]$.

We simply continue as before:

$$\begin{aligned} [L_z, L_x] &= [L_z, YP_z - ZP_y] = [L_z, Y]P_z + Y[L_z, P_z] - [L_z, Z]P_y - Z[L_z, P_y] \\ &= -i\hbar XP_z + 0 - 0 - Z(-i\hbar P_x) = i\hbar(ZP_x - XP_z) = i\hbar L_y, \\ [L_z, L_y] &= [L_z, ZP_x - XP_z] = [L_z, Z]P_x + Z[L_z, P_x] - [L_z, X]P_z - X[L_z, P_z] \\ &= 0 + Zi\hbar P_y - i\hbar YP_z - 0 = i\hbar(ZP_y - YP_z) = -i\hbar L_x. \end{aligned}$$

5. [5] Prove the parity operator Π , defined by (3.40) is both Hermitian and unitary.

To show it is Hermitian, we must show that $\langle \phi | \Pi | \psi \rangle^* = \langle \psi | \Pi | \phi \rangle$, so

$$\begin{aligned} \langle \phi | \Pi | \psi \rangle^* &= \left[\iiint d^3\mathbf{r} \phi^*(\mathbf{r}) \psi(-\mathbf{r}) \right]^* = \iiint d^3\mathbf{r} \psi^*(-\mathbf{r}) \phi(\mathbf{r}) = \iiint d^3\mathbf{r} \psi^*(\mathbf{r}) \phi(-\mathbf{r}) \\ &= \langle \psi | \Pi | \phi \rangle \end{aligned}$$

Now that we know it is Hermitian, we can take advantage of this to show that

$$\Pi^\dagger \Pi \psi(\mathbf{r}) = \Pi^2 \psi(\mathbf{r}) = \Pi \psi(-\mathbf{r}) = \psi(\mathbf{r}).$$

Since this is true for all wave functions, it follows that $\Pi^\dagger \Pi = 1$.

6. [15] Consider the Hermitian matrix: $H = E_0 \begin{pmatrix} 0 & 3i & 0 \\ -3i & 8 & 0 \\ 0 & 0 & 8 \end{pmatrix}$

(a) [10] Find all three eigenvalues and eigenvectors of H .

We note first that it is block-diagonal, as I have sketched in with dashed lines in the problem itself, reducing the matrix to a 2×2 matrix and a trivial 1×1 matrix:

$$H_2 = E_0 \begin{pmatrix} 0 & 3i \\ -3i & 8 \end{pmatrix} \quad \text{and} \quad H_1 = E_0 (8)$$

The matrix H_1 has eigenvalue $8E_0$, and eigenvector (1), which makes it trivial. The eigenvalues of matrix H_2 can be found using the characteristic equation

$$\begin{aligned} 0 &= \det(H_2 - \lambda \mathbf{1}) = \begin{vmatrix} -\lambda & 3iE_0 \\ -3iE_0 & 8E_0 - \lambda \end{vmatrix} = \lambda^2 - 8\lambda E_0 - (3i)(-3i)E_0^2 = \lambda^2 - 8\lambda E_0 - 9E_0^2 \\ &= (\lambda - 9E_0)(\lambda + E_0) \end{aligned}$$

This has solutions $\lambda = 9E_0$ and $\lambda = -E_0$. To find each of these values, we put in an arbitrary vector and solve the eigenvalue equation. For example, for $\lambda = 9E_0$, we have

$$\begin{aligned} \begin{pmatrix} 0 & 3iE_0 \\ -3iE_0 & 8E_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} &= 9E_0 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \\ \begin{pmatrix} 3i\beta \\ -3i\alpha + 8\beta \end{pmatrix} &= \begin{pmatrix} 9\alpha \\ 9\beta \end{pmatrix}. \end{aligned}$$

The first of these equations implies $\beta = -3i\alpha$; if we plug this into the second, we find that it is also automatically satisfied. We also want the eigenvector normalized, so

$$1 = |\alpha|^2 + |\beta|^2 = 10|\alpha|^2$$

We have an arbitrary phase to choose; if we pick α to be real and positive, $\alpha = 1/\sqrt{10}$, and we have the eigenvector

$$|9E_0\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ -3i \end{pmatrix}$$

For the other eigenvector, we have

$$\begin{pmatrix} 0 & 3iE_0 \\ -3iE_0 & 8E_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -E_0 \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

$$\begin{pmatrix} 3i\beta \\ -3i\alpha + 8\beta \end{pmatrix} = \begin{pmatrix} -\alpha \\ -\beta \end{pmatrix}$$

Both equations imply $\beta = i\alpha/3$. Our normalization condition becomes

$$1 = |\alpha|^2 + |\beta|^2 = \frac{10}{9}|\alpha|^2$$

Once again we pick α to be real and positive, $\alpha = 3/\sqrt{10}$, and we have the eigenvector

$$|-E_0\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ i \end{pmatrix}$$

Returning to the full three-dimensional space, our eigenvectors are

$$|-E_0\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ i \\ 0 \end{pmatrix}, \quad |9E_0\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ -3i \\ 0 \end{pmatrix}, \quad |8E_0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Your answers might be slightly different, in that the phases could be different, or the eigenvectors could be listed in a different order.

(b) [5] Construct the unitary matrix V which diagonalizes H . Check explicitly that $V^\dagger V = 1$ and $V^\dagger H V = H'$ is real and diagonal.

The unitary matrix V just consists of the eigenvectors listed in any order, so we have

$$V = \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} & 0 \\ \frac{i}{\sqrt{10}} & -\frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Your answer could be different, in that the columns could come in a different order, and each column could be multiplied by an arbitrary phase.

We have ahead of us some boring matrix multiplication.

$$\begin{aligned} V^\dagger V &= \begin{pmatrix} \frac{3}{\sqrt{10}} & -\frac{i}{\sqrt{10}} & 0 \\ \frac{1}{\sqrt{10}} & \frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} & 0 \\ \frac{i}{\sqrt{10}} & -\frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{9}{10} + \frac{1}{10} & \frac{3}{10} - \frac{3}{10} & 0 \\ \frac{3}{10} - \frac{3}{10} & \frac{1}{10} + \frac{9}{10} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ V^\dagger H V &= E_0 \begin{pmatrix} \frac{3}{\sqrt{10}} & -\frac{i}{\sqrt{10}} & 0 \\ \frac{1}{\sqrt{10}} & \frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 3i & 0 \\ -3i & 8 & 0 \\ 0 & 0 & 8 \end{pmatrix} \begin{pmatrix} \frac{3}{\sqrt{10}} & \frac{1}{\sqrt{10}} & 0 \\ \frac{i}{\sqrt{10}} & -\frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= E_0 \begin{pmatrix} \frac{3}{\sqrt{10}} & -\frac{i}{\sqrt{10}} & 0 \\ \frac{1}{\sqrt{10}} & \frac{3i}{\sqrt{10}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -\frac{3}{\sqrt{10}} & \frac{9}{\sqrt{10}} & 0 \\ -\frac{i}{\sqrt{10}} & -\frac{27i}{\sqrt{10}} & 0 \\ 0 & 0 & 8 \end{pmatrix} = E_0 \begin{pmatrix} -\frac{9}{10} - \frac{1}{10} & \frac{27}{10} - \frac{27}{10} & 0 \\ -\frac{3}{10} + \frac{3}{10} & \frac{9}{10} + \frac{81}{10} & 0 \\ 0 & 0 & 8 \end{pmatrix} \\ &= E_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 9 & 0 \\ 0 & 0 & 8 \end{pmatrix} \end{aligned}$$

As you can see, $V^\dagger V = 1$ and $V^\dagger H V$ is real and diagonal (and has the eigenvalues on its diagonal).