THE UNIVERSITY OF QUEENSLAND
SCHOOL OF MATHEMATICS AND PHYSICS
PHYS2041 – Quantum Physics

Tutorial 7 Solutions

Problem 7.1

We are given that $|\psi_n\rangle$ forms an orthonormal basis. We are free to expand our state (we also refer to this object as a ket, or vector) *any* complete basis, but it will be convenient to choose this basis,

$$|\Psi\rangle = \sum_m c_m |\psi_m\rangle \tag{1}$$

where c_n are the (complex) expansion coefficients. Because $|\psi_n\rangle$ are orthogonal we have $\langle\psi_n|\psi_m\rangle = \delta_{m,n}$, where $\delta_{m,n}$ is the Kronecker delta-function. This gives us a formula for c_n,

$$\begin{aligned}
\langle\psi_n|\Psi\rangle &= \sum_m c_m \langle\psi_n|\psi_m\rangle && (2)\\
&= \sum_m c_m \delta_{m,n} && (3)\\
&= c_n, && (4)
\end{aligned}$$

i.e., $c_n = \langle\psi_n|\Psi\rangle$.

With this in mind, let's think about how this operator acts on an arbitrary ket, $|\Psi\rangle$. We have,

$$\begin{aligned}
&\left(\sum_n |\psi_n\rangle\langle\psi_n|\right)|\Psi\rangle && (5)\\
&= \sum_n |\psi_n\rangle\langle\psi_n|\Psi\rangle && (6)\\
&= \sum_n c_n|\psi_n\rangle \text{ (using Eq.4)} && (7)\\
&= |\Psi\rangle \text{ (using Eq.1).} && (8)
\end{aligned}$$

Thus, we see that the action of the operator is to simply return the original ket $|\Psi\rangle$, which was arbitrary. In other words, this operator maps any ket to itself - and so it makes sense to call $\sum_n |\psi_n\rangle\langle\psi_n| = \hat{1}$ the identity operator!

Problem 7.2

In the hint for this question we are told that an operator is characterised by its action on all possible vectors (or kets). So as with the previous question, let's start with an arbitrary ket

$|\Psi\rangle$, which we'll choose to write in the eigenbasis (i.e. the set of all energy eigenstates) of the Hamiltonian operator $\hat{H}$

$$|\Psi\rangle = \sum_n c_n|\psi_n\rangle \tag{9}$$

where

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle. \tag{10}$$

Remember, we are free to expand any vector in any complete basis. We are simply choosing to use this basis because it'll help us when we try and explore the action of $\hat{H}$ on $|\Psi\rangle$. The action of $\hat{H}$ on an arbitrary ket $|\Psi\rangle$ is

$$\begin{align}
\hat{H}|\Psi\rangle &= \sum_n c_n\hat{H}|\psi_n\rangle \tag{11}\\
&= \sum_n c_n E_n|\psi_n\rangle \text{ (using Eq.10)} \tag{12}\\
&= \sum_n \langle\psi_n|\Psi\rangle E_n|\psi_n\rangle \text{ (using Eq.4)} \tag{13}\\
&= \left(\sum_n E_n|\psi_n\rangle\langle\psi_n|\right)|\Psi\rangle. \tag{14}
\end{align}$$

In the final line we have made use of the fact that $\langle\psi_n|\Psi\rangle$ is a scalar, which can be freely moved around. All of this implies

$$\hat{H} = \sum_n E_n|\psi_n\rangle\langle\psi_n|, \tag{15}$$

which was the result to be shown.

At no point did we actually have to assume anything about the operator $\hat{H}$ (except that it has well-defined eigenvectors and eigenvalues), which means that this result is true for any operator, not just $\hat{H}$. This is called the spectral decomposition because the set of eigenvalues of an operator is called its spectrum (the language comes from the atomic spectra).

Problem 7.3 [FOR ASSIGNMENT 4; max 10 points]

(a) The time-dependent Schrödinger equation holds for state vectors (or kets) just as it does for wavefunctions, i.e.

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle. \tag{16}$$

To show that

$$|\Psi(t)\rangle = \sum_n c_n|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{17}$$

is a solution (where $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$), we can just substitute this into the time-dependent Schrödinger equation, and show that the right-hand side (RHS) is equal to the left-hand side

(LHS). The LHS is easy to evaluate,

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\sum_n c_n|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{18}$$

$$= i\hbar\sum_n c_n|\psi_n\rangle\frac{\partial}{\partial t}e^{-i\frac{E_n}{\hbar}t} \tag{19}$$

$$= i\hbar\sum_n c_n|\psi_n\rangle\left(-i\frac{E_n}{\hbar}\right)e^{-i\frac{E_n}{\hbar}t} \tag{20}$$

$$= \sum_n c_n E_n|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t}, \tag{21}$$

where in the second line we have made use of the fact that c_n do not depend on time. To evaluate the RHS, we have

$$\hat{H}|\Psi\rangle = \sum_n c_n\hat{H}|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{22}$$

$$= \sum_n c_n\left(\sum_m E_m|\psi_m\rangle\langle\psi_m|\right)|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{23}$$

where in the second line we have used the spectral decomposition for $\hat{H}$ from the previous question. Notice that we have used a different index on the two sums, since they are independent. Remember that $|\psi_n\rangle$ are the eigenvectors of $\hat{H}$, which are orthonormal. Continuing the calculation,

$$\hat{H}|\Psi\rangle = \sum_n\sum_m c_n E_m|\psi_m\rangle\langle\psi_m|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{24}$$

$$= \sum_n\sum_m c_n E_m|\psi_m\rangle\delta_{m,n}e^{-i\frac{E_n}{\hbar}t} \tag{25}$$

$$= \sum_n c_n E_n|\psi_n\rangle e^{-i\frac{E_n}{\hbar}t} \tag{26}$$

$$= i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle \text{ (Eq.21)}. \tag{27}$$

Thus we have shown that the LHS=RHS, and so $|\Psi(t)\rangle$ solves the time-dependent Schrödinger equation.

This is an illustration of why the eigenstates of $\hat{H}$ are so important in quantum mechanics. Of course we could choose to write the state in any basis, but Eq. (25) will only follow if we use $\hat{H}$ eigenstates.

(b) Although we aren't told what the Hamiltonian for this system is, we can write the solution in terms of energies E_n by making use of Eq. (17). We know that the nth coefficient is $c_n = \langle\psi_n|\Psi(0)\rangle$ [see Eq. (4)]. We are given every c_n, so it is simply a matter of writing out the state,

$$|\Psi(t)\rangle = \frac{1}{\sqrt{6}}|\psi_6\rangle e^{-i\frac{E_6}{\hbar}t} - \frac{i}{\sqrt{2}}|\psi_{17}\rangle e^{-i\frac{E_{17}}{\hbar}t} + \frac{1}{\sqrt{3}}|\psi_{271}\rangle e^{-i\frac{E_{271}}{\hbar}t}. \tag{28}$$

It's always good to check that the state is normalised, $|\langle\Psi(t)|\Psi(t)\rangle|^2 = |1/\sqrt{6}|^2 + |-i/\sqrt{2}|^2 + |1/\sqrt{3}|^2 = 1$.

Problem 7.4 **[FOR ASSIGNMENT 4; max 10 points]** The trick here is to multiply by the identity (given in Problem 7.1) operator *twice*, being careful to use different indices on the independent sums,

$$\begin{aligned}
\hat{A} &= \hat{1}\hat{A}\hat{1} && (29)\\
&= \left(\sum_m |\psi_m\rangle\langle\psi_m|\right)\hat{A}\left(\sum_n |\psi_n\rangle\langle\psi_n|\right) && (30)\\
&= \sum_m\sum_n |\psi_m\rangle\langle\psi_m|\hat{A}|\psi_n\rangle\langle\psi_n| && (31)\\
&= \sum_m\sum_n \langle\psi_m|\hat{A}|\psi_n\rangle|\psi_m\rangle\langle\psi_n| && (32)\\
&= \sum_m\sum_n A_{m,n}|\psi_m\rangle\langle\psi_n| && (33)
\end{aligned}$$

where

$$A_{m,n} = \langle\psi_m|\hat{A}|\psi_n\rangle \tag{34}$$

are called the *matrix elements* of $\hat{A}$, which are scalar. One way to understand this result is to think about the matrix elements of a single basis matrix, for instance

$$|\psi_1\rangle\langle\psi_1| = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad |\psi_1\rangle\langle\psi_2| = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad |\psi_2\rangle\langle\psi_1| = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{35}$$

etc. Hopefully you can imagine that summing up every one of these, multiplied by the relevant scalar $A_{m,n}$ will construct the matrix $\hat{A}$. Although in this assignment we are using the convention that $|\psi_n\rangle$ are the eigenstates of the Hamiltonian operator, the result we have derived here is true in any basis (think, did we need to use $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ anywhere?).

If we were to calculate the matrix elements of the Hamiltonian matrix using the energy eigenstates $|\psi_n\rangle$ as the basis, we would find that the matrix elements are $H_{m,n} = \langle\psi_m|\hat{H}|\psi_n\rangle = E_n\langle\psi_m|\psi_n\rangle = E_n\delta_{m,n}$, which recovers the spectral decomposition from Problem 7.2. Because the $\delta_{m,n}$ would collapse one of the sums the resultant matrix would be diagonal. Notice that the matrix elements of the identity operator are simply $1_{m,n} = \delta_{m,n}$, which would produce a matrix that is zero everywhere, except with ones on the diagonal – this is precisely the identity matrix!