Physics 580 | **Quantum Mechanics I** | Prof. P. M. Goldbart

Handout 10 | `webusers.physics.illinois.edu/~goldbart/` | 3135 (& 2115) ESB

5 October 2010 | Homework 6 | University of Illinois

1) Periodic functions: In this question we shall consider the LVS formed by complex square-integrable functions on the interval $[0, 2\pi]$ with periodic boundary conditions

$$f(0) = f(2\pi), \qquad f'(0) = f'(2\pi),$$

where f' denotes df/dx. By square integrable we mean that $\int_0^{2\pi} dx|f(x)|^2 < \infty$. Answer, with explanations, the following questions.

a) Is the function $f(x) = \exp(ix/2)$ in this space?

b) Is the function $f(x) = x(2\pi - x)$ in this space?

c) Write an arbitrary ket $|f\rangle$ in this space in terms of the basis $\{|x\rangle\}$ and the components $f(x)$.

d) Evaluate $\langle x|f\rangle$ in terms of $f(x)$.

For an operator Ω to be hermitean on a certain infinite-dimensional linear vector: (i) Ω must be formally self-adjoint, *i.e.*, up to boundary terms it must satisfy

$$\langle g|\Omega|f\rangle = \langle f|\Omega|g\rangle^*;$$

and (ii) the boundary conditions must be self-adjoint, so that both functions f and g come from the same function space (*i.e.*, satisfy the same boundary conditions). Boundary conditions are said to be self-adjoint if their application to f, together with the demand that the boundary term vanishes, obliges g to satisfy identical boundary conditions. We now apply these ideas to the operator T.

e) An operator T is defined by its action on arbitrary kets $|f\rangle$ in the following way:

$$\langle x|T|f\rangle = -\frac{d^2}{dx^2} f(x).$$

Here, $|f\rangle = \int_0^{2\pi} dx\, f(x)|x\rangle$. With the boundary conditions on $f(x)$ given above, discuss the hermicity of the operator T. Do you expect to find: (i) that all eigenvalues of T are real; and (ii) that its eigenkets provide an orthonormal basis for the LVS?

f) Repeat part (e) but now consider the boundary conditions

$$f(0) = f(2\pi) = 0.$$

Can you think of any other boundary conditions for which T is hermitean?

g) Return to the case of periodic boundary conditions. Resolve the eigenproblem,

$$T|\phi_m\rangle = t_m|\phi_m\rangle,$$

on to the basis $\{|x\rangle\}$. Write this eigenproblem as a differential equation for the complex-valued function $\phi_m(x)$.

h) By demonstrating that the functions

$$\phi_m(x) = \frac{e^{imx}}{\sqrt{2\pi}} \qquad \text{for} \quad \text{integer} \quad m$$

i) satisfy the differential equation;
ii) satisfy the boundary conditions;
iii) are normalised; and
iv) yield eigenvalues m^2;

show that the kets $|\phi_m\rangle$ solve the T-eigenproblem.

i) From your experience with Fourier series, do you suspect that the eigenfunctions are complete (*i.e.*, span the LVS)?

j) Prove the orthogonality relation $\langle\phi_m|\phi_n\rangle = \delta_{nm}$ by using the explicit representation for $\langle x|\phi_m\rangle$.

Now that we have two bases, $\{|x\rangle\}$ and $\{|\phi_m\rangle\}$, we can expand in either one:

$$|f\rangle = \int_0^{2\pi} dx\, f(x)\,|x\rangle \;=\; \sum_{m=-\infty}^{\infty} f_m\,|\phi_m\rangle.$$

k) Write $f(x)$ and f_m as inner products of something with $|f\rangle$.

l) By inserting a resolution of the identity, prove that

$$f_m = \langle\phi_m|f\rangle = \int_0^{2\pi} dx\, \langle\phi_m|x\rangle\,\langle x|f\rangle = \int_0^{2\pi} dx\, \phi_m(x)^*\, f(x).$$

Now think about the following statement: Finding the Fourier coefficients f_m, given the function $f(x)$, is an example of changing the basis from $\{|x\rangle\}$ to $\{|\phi_m\rangle\}$. (You do not need to write anything down for this last part.)

m) Evaluate the matrix elements in the $\{|x\rangle\}$-basis of the unitary operator which implements this change in basis?

2) Normalisation: Consider the LVS of complex-valued functions $\phi(x)$ on the real line $(-\infty < x < \infty)$. Restrict your attention to the subset of these functions that can be normalised either

i) to unity or
ii) to the Dirac delta function.

We call this subset the physical Hilbert space.

a) Can the following ket be normalised to unity:

$$|\phi_1\rangle = A \int_{-\infty}^{\infty} dx \, \exp\left(-x^2/4\right) |x\rangle?$$

[Hint: $\int_{-\infty}^{\infty} dx \, \exp(-x^2/2) = \sqrt{2\pi}$; what is the necessary A?]

b) Can the following ket be normalised to the Dirac delta function

$$|\phi_2\rangle = B \int_{-\infty}^{\infty} dx \, \frac{\mathrm{e}^{ikx}}{\sqrt{2\pi}} |x\rangle?$$

The position operator X acts on kets $\{|y\rangle\}$ such that $X|y\rangle = y|y\rangle$, where y lives on the real line.

c) Write down the matrix element $\langle z|X|y\rangle$.
d) Write down the matrix element $\langle z|X|\phi\rangle$ in terms of $\phi(z) = \langle z|\phi\rangle$.
e) By noting that y is real, discuss whether the operator X is hermitean.
f) The operator P acts on general kets $\{|\phi\rangle\}$ such that $\langle x|P|\phi\rangle = -i\hbar d\phi/dx$. By using integration by parts, and neglecting boundary terms, show that P is self-adjoint, *i.e.*, that

$$\langle\psi|P|\phi\rangle^* = \langle\phi|P|\psi\rangle.$$

g) Show that

$$\begin{aligned} \langle y|XP|\phi\rangle &= -i\hbar y \frac{d}{dy}\phi(y), \\ \langle y|PX|\phi\rangle &= -i\hbar \frac{d}{dy} y\phi(y). \end{aligned}$$

h) Hence show that $\langle y|[X,P]|\phi\rangle = i\hbar\langle y|\phi\rangle$ and, thus, that $[X,P] = i\hbar \mathrm{I}$.

3) Probability densities and currents: Consider a particle of mass m moving in three dimensions with momentum $\mathbf{p}$, position $\mathbf{x}$, and hamiltonian $h(\mathbf{x}, \mathbf{p})$ given by

$$h(\mathbf{x}, \mathbf{p}) = \frac{|\mathbf{p}|^2}{2m} + U(\mathbf{x}).$$

a) Suppose the state of the particle is described by a normalised wave function $\psi(\mathbf{x})$. In wave mechanics, the probability density $n(\mathbf{x})$ is given by

$$n(\mathbf{x}) = |\psi(\mathbf{x})|^2.$$

Show, by using the time-dependent Schrödinger *wave* equation (*i.e.*, a partial differential equation) that the probability current,

$$\mathbf{j}(\mathbf{x}) = \frac{\hbar}{2im}(\psi^* \nabla \psi - \psi \nabla \psi^*),$$

is a conserved quantity.

b) We will now examine the *bra and ket* version of part (a). Suppose the six operators, $\mathbf{X}$ and $\mathbf{P}$, are the position and momentum operators for our particle, the state of which is described by the normalised state vector $|\psi\rangle$. Show that the probability density in part (a), $n(\mathbf{x})$, is given by the expectation value in the state $|\psi\rangle$ of the probability density operator

$$N(\mathbf{x}) \equiv \delta(\mathbf{x} - \mathbf{X}) = |\mathbf{x}\rangle\langle\mathbf{x}|.$$

Notice that $\mathbf{x}$ enters here as a *parameter*: there is one operator for each position $\mathbf{x}$. This operator N is the *position-basis* case of the general probability projection operator, introduced in class.

Show that the probability current in part (a) is the expectation value in the state $|\psi\rangle$ of the symmetrised probability current operator

$$\mathbf{J}(\mathbf{y}) \equiv \frac{1}{2m}\{\mathbf{P}\,\delta(\mathbf{y} - \mathbf{X}) + \delta(\mathbf{y} - \mathbf{X})\,\mathbf{P}\}.$$

Show that

$$\frac{\partial}{\partial t}\langle\psi|N(\mathbf{x})|\psi\rangle + \nabla \cdot \langle\psi|\mathbf{J}(\mathbf{x})|\psi\rangle = 0,$$

and, hence, that probability is conserved.