

**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

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

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.

- Is the function  $f(x) = \exp(ix/2)$  in this space?
- Is the function  $f(x) = x(2\pi - x)$  in this space?
- Write an arbitrary ket  $|f\rangle$  in this space in terms of the basis  $\{|x\rangle\}$  and the components  $f(x)$ .
- Evaluate  $\langle x|f\rangle$  in terms of  $f(x)$ .

For an operator  $\Omega$  to be hermitean on a certain infinite-dimensional linear vector: (i)  $\Omega$  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  $T$ .

- 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?

- 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?

- 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

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

- 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:

$$|\phi_1\rangle = A \int_{-\infty}^{\infty} dx \exp\left(-\frac{1}{4}x^2\right) |x\rangle?$$

[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

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

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  $[X, P] = i\hbar I$ .

**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.