Problem Set 1: Quantum and Math Review
Graduate Quantum I
Physics 6572
James Sethna
Due Monday Aug 27 (Five days from now!)
Last correction at August 24, 2012, 9:23 pm

Reading

Sakurai and Napolitano, sections 1.1-1.5

Other Resources

Summary of Quantum Mechanics, pp. 1-14 from
The Quantum Mechanics Solver, Jean-Louise Basdevant and Jean Dalibard

These exercises review and introduce mathematics and physics definitions, notation, and relations that will be important to the rest of the course. The should not involve long calculations.

1.1 **Quantum Notation.** (Notation) ②

For each entry in the first column, match the corresponding entries in the second and third column.

Schrödinger	*Dirac*	*Physics*
$\psi(x)$	*A.* $\langle\psi\|x\rangle p/2m\langle x\|\psi\rangle - \langle x\|\psi\rangle p/2m\langle\psi\|x\rangle$	*I. The number one*
$\psi^*(x)$	*B. Ket* $\|\psi\rangle$ *in position basis, or* $\langle x\|\psi\rangle$	*II. Probability density at* x
$\|\psi(x)\|^2$	*C. Bra* $\langle\psi\|$ *in position basis, or* $\langle\psi\|x\rangle$	*III. Probability* ψ *is in state* ϕ
$\int \phi^*(x)\psi(x)\mathrm{d}x$	*D.* $\langle\psi\|x\rangle\langle x\|\psi\rangle$	*IV. Amplitude of* ψ *at* x
$\|\int \phi^*(x)\psi(x)\mathrm{d}x\|^2$	*E. Braket* $\langle\phi\|\psi\rangle$	*V. Amplitude of* ψ *in state* ϕ
$\int \|\psi(x)\|^2\mathrm{d}x$	*F.* $\langle\psi\|\psi\rangle$	*VI. Current density*
$(\hbar/2m\mathrm{i})(\psi^*\nabla\psi - \psi\nabla\psi^*)$	*G.* $\langle\psi\|\phi\rangle\langle\phi\|\psi\rangle$	*VII. None of these.*

1.2 **Rotation Matrices.** (Math,$\times\mathbb{1}$) ②

A rotation matrix R takes an orthonormal basis $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ into another orthonormal triad $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$, $\hat{\mathbf{w}}$, with $\hat{\mathbf{u}} = R\hat{\mathbf{x}}$, $\hat{\mathbf{v}} = R\hat{\mathbf{y}}$, and $\hat{\mathbf{w}} = R\hat{\mathbf{z}}$.

(a) Which is another way to write the matrix R? *I.* $R = \begin{pmatrix} u_1v_1 + v_1w_1 + w_1u_1 & \cdots \\ \cdots & \end{pmatrix}$

II. $R = \begin{pmatrix} (& \hat{\mathbf{u}} &) \\ (& \hat{\mathbf{v}} &) \\ (& \hat{\mathbf{w}} &) \end{pmatrix}$; *III.* $R = \left(\begin{pmatrix} \hat{\mathbf{u}} \end{pmatrix} \quad \begin{pmatrix} \hat{\mathbf{v}} \end{pmatrix} \quad \begin{pmatrix} \hat{\mathbf{w}} \end{pmatrix} \right)$; *IV.* $R = \hat{\mathbf{u}}\otimes\hat{\mathbf{v}} + \hat{\mathbf{v}}\otimes\hat{\mathbf{w}} + \hat{\mathbf{w}}\otimes\hat{\mathbf{u}}$

Rotation matrices are to real vectors what unitary transformations (common in quantum mechanics) are to complex vectors. A unitary transformation satisfies $U^\dagger U = \mathbb{1}$, where the 'dagger' gives the complex conjugate of the transpose, $U^\dagger = (U^T)^*$. Since R is real, $R^\dagger = R^T$.

(b) Argue that $R^T R = \mathbb{1}$.

Thus R is an *orthogonal* matrix, with transpose equal to its inverse.

(c) In addition to (b), what other condition do we need to know that R is a proper rotation (i.e., in $SO(3)$), and not a rotation-and-reflection with determinant -1?
(I) $\hat{\mathbf{u}}$, $\hat{\mathbf{v}}$, *and* $\hat{\mathbf{w}}$ *must form a right-handed triad (presuming as usual that* $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, *and* $\hat{\mathbf{z}}$ *are right-handed),*
(II) $\hat{\mathbf{u}} \cdot \hat{\mathbf{v}} \times \hat{\mathbf{w}} = 1$
(III) $\hat{\mathbf{w}} \cdot \hat{\mathbf{u}} \times \hat{\mathbf{v}} = 1$
(IV) All of the above

One of the most useful tricks in quantum mechanics is multiplying by one. The operator $|k\rangle\langle k|$ can be viewed as a projection operator: $|k\rangle\langle k|\psi\rangle$ is the part of $|\psi\rangle$ that lies along direction $|k\rangle$. If k labels a complete set of orthogonal states (say, the eigenstates of the Hamiltonian), then the original state can be reconstructed by adding up the components along the different directions: $|\psi\rangle = \sum_k |k\rangle\langle k|\psi\rangle$. Hence the identity operator $\mathbb{1} = \sum_k |k\rangle\langle k|$. We'll use this to derive the path-integral formulation of quantum mechanics, for example. Let's use it here to derive the standard formula for rotating matrices.

Under a change of basis R, a matrix A transforms to $R^T A R$. We are changing from the basis $\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \hat{\mathbf{x}}_3 = |x_i\rangle$ to the basis $|u_j\rangle$, with $|u_n\rangle = R|x_n\rangle$. Since $|u_j\rangle = R|x_j\rangle$, we know $\langle x_i|u_j\rangle = \langle x_i|R|x_j\rangle = R_{ij}$, and similarly $\langle u_i|x_j\rangle = R^T_{ij}$. Let the original components of the operator $\mathbb{A}$ be $A_{k\ell} = \langle x_k|A|x_\ell\rangle$ and the new coordinates be $A'_{ij} = \langle u_i|A|u_j\rangle$.

(d) Multipling by one twice into the formula for A': $A'_{ij} = \langle u_i|\mathbb{1}A\mathbb{1}|u_j\rangle$ *and expanding the first and second identities in terms of* x_k *and* x_ℓ*, derive the matrix transformation formula* $A'_{ij} = R^T_{ik} A_{k\ell} R_{\ell j} = R^T A R$*, where we use the Einstein summation convention over repeated indices..*

1.3 **Eigen Stuff.** (Math,$\times\mathbb{1}$) ②

Consider an operator for a two-state system $O = \begin{pmatrix} 0 & -4 \\ -4 & 6 \end{pmatrix}$ Its eigenvectors are $|e_1\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ and $|e_2\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} -1 \\ 2 \end{pmatrix}$

(a) What are the associated eigenvalues o_1 *and* o_2*?*

(b) Use $|e_1\rangle$ *and* $|e_2\rangle$ *to construct a rotation matrix* R *that diagonalizes* O*, so* $R^T O R = \begin{pmatrix} o_1 & 0 \\ 0 & o_2 \end{pmatrix}$. (Hint: See problem 2(a). We want R to rotate the axes into $\hat{\mathbf{u}} = |e_1\rangle$ and $\hat{\mathbf{v}} = |e_2\rangle$.) *What angle does* R *rotate by?*

(c) Assume that the system is in a state $|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ *Decompose* $|L\rangle$ *into the eigenvectors of* O. (Hint: As in exercise 2(d), multiplying $|L\rangle$ by one is useful.) *If the observable corresponding to the operator* O *is measured for state* $|L\rangle$*, what is the probability of finding the value* o_1*? Does the probability of finding either* o_1 *or* o_2 *sum to one?*

1.4 **Trace.** (Math,$\times\mathbb{1}$) ②

The trace of a matrix A is $Tr(A) = \sum_i A_{ii} = A_{ii}$ where the last form makes use of the *Einstein summation convention.*

(a) Show the trace has a cyclic invariance: $Tr(ABC) = Tr(BCA)$. (Hint: write it out as a sum over components. Matrices don't commute, but products of components of matrices are just numbers, and do commute.) *Is* $Tr(ABC) = Tr(ACB)$ *in general?*

Remember from exercise 2(b) that a rotation matrix R has its inverse equal to its transpose, so $R^T R = \mathbb{1}$, and that a matrix A transforms into $R^T A R$ under rotations.

(b) Using the cyclic invariance of the trace, show that the trace is invariant under rotations.

Rotation invariance is the primary reason that the trace is so important in mathematics and physics.