Problem Set 2: Interferometers & Random Matrices
Graduate Quantum I
Physics 6572

James Sethna

Due Friday Sept. 5

Last correction at August 28, 2014, 8:32 pm

Potentially useful reading

Sakurai and Napolitano, sections 1.5 (Rotation),
Schumacher & Westmoreland chapter 2

2.1 **Commutation of functions of x and p** (Sakurai and Napolitano, exercise 1.29).

(a) *On page 247, Gottfried (1966) states that*

$$[x_i, G(\mathbf{p})] = \mathrm{i}\hbar\frac{\partial G}{\partial p_i}, \qquad [p_i, F(\mathbf{x})] = -\mathrm{i}\hbar\frac{\partial F}{\partial x_i} \tag{1}$$

can be "easily derived" from the fundamental commutation relations for all functions of F and G that can be expressed as a power series in their arguments. Verify this statement.

(b) *Evaluate $[x^2, p^2]$ in the case of one dimension. Compare your result with the classical Poisson bracket $\{x^2, p^2\}_{\mathrm{classical}}$.*

2.2 **Buckyball wavelengths** (Schumacher & Westmoreland problem 1.4).

In 1999, a research group at the University of Vienna was able to observe quantum interference in a beam of C_{60} molecules. C_{60} is called *buckminsterfullerene*, and the soccerbal-shaped C_{60} molecules are sometimes called *buckyballs*. A buckyball molecule has a mass of about 1.2×10^{-24} kg.

(a) *The buckyball wavelength in the experiment was about 3pm. How fast were the molecules moving?*

(b) *What would be the wavelength of an electron moving at the same speed?*

2.3 **Adiabatic theorem** (Schumacher & Westmoreland problem 2.5).

Consider a spin-1/2 particle passing through a series of spin filters (See Figure 2.13 on p.35 of Schumacher & Westmoreland). Now, however, there are 13 filters (numbered 0 through 12). The n-th filter selects for the state $|n_+\rangle$, the $+\hbar/2$ basis state for a measurement of spin along an axis in the xz-plane an angle $n\pi/12$ from z. From Eq. 2.35, we can write

$$|n_+\rangle = \cos\frac{n\pi}{24}\,|z_+\rangle + \sin\frac{n\pi}{24}\,|z_-\rangle. \tag{2}$$

What is the probability that a spin-1/2 particle, initially in the state $|z_+\rangle$, will pass all 13 filters?

2.4 **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. $R = \Big(\big(\hat{\mathbf{u}}\big)\ \big(\hat{\mathbf{v}}\big)\ \big(\hat{\mathbf{w}}\big)\Big)$;

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..

2.5 **Random matrix theory.**[1] (Mathematics, Quantum) ③

One of the most active and unusual applications of ensembles is *random matrix theory*, used to describe phenomena in nuclear physics, mesoscopic quantum mechanics, and wave phenomena. Random matrix theory was invented in a bold attempt to describe the statistics of energy level spectra in nuclei. In many cases, the statistical behavior of systems exhibiting complex wave phenomena—almost any correlations involving eigenvalues and eigenstates—can be quantitatively modeled using ensembles of matrices with completely random, uncorrelated entries!

To do this exercise, you will need to find a software environment in which it is easy to (i) make histograms and plot functions on the same graph, (ii) find eigenvalues of matrices, sort them, and collect the differences between neighboring ones, and (iii) generate symmetric random matrices with Gaussian and integer entries. Mathematica, Matlab, Octave, and Python are all good choices. For those who are not familiar with one of these packages, I will post hints on how to do these three things under 'Random matrix theory' in the computer exercises section of the book web site (http://pages.physics.cornell.edu/~myers/teaching/ComputationalMethods/ComputerExercises/RandomMatrixTheory/RandomMatrixTheory.html).

The most commonly explored ensemble of matrices is the Gaussian orthogonal ensemble (GOE). Generating a member H of this ensemble of size $N \times N$ takes two steps.

- Generate an $N \times N$ matrix whose elements are independent random numbers with Gaussian distributions of mean zero and standard deviation $\sigma = 1$.
- Add each matrix to its transpose to symmetrize it.

As a reminder, the Gaussian or normal probability distribution of mean zero gives a random number x with probability

$$\rho(x) = \frac{1}{\sqrt{2\pi}\sigma} \mathrm{e}^{-x^2/2\sigma^2}. \tag{3}$$

One of the most striking properties that large random matrices share is the distribution of level splittings.

(a) *Generate an ensemble with* $M = 10000$ *or more GOE matrices of size* $N = 2$, 4, *and* 10. *Find the eigenvalues* λ_n *of each matrix, sorted in increasing order. Find the difference between neighboring eigenvalues* $\lambda_{n+1} - \lambda_n$, *for* n, *say, equal to*[2] $N/2$. *Plot a histogram of these eigenvalue splittings divided by the mean splitting, with bin size small enough to see some of the fluctuations.* (Hint: Debug your work with $M = 10$, and then change to $M = 10000$.)

What is this dip in the eigenvalue probability near zero? It is called *level repulsion*.

[1] This exercise was developed with the help of Piet Brouwer.

[2] Why not use all the eigenvalue splittings? The mean splitting can change slowly through the spectrum, smearing the distribution a bit.

For $N = 2$ the probability distribution for the eigenvalue splitting can be calculated pretty simply. Let our matrix be $M = \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right)$.

(b) *Show that the eigenvalue difference for M is $\lambda = \sqrt{(c-a)^2 + 4b^2} = 2\sqrt{d^2 + b^2}$ where $d = (c-a)/2$, and the trace $c+a$ is irrelevant. Ignoring the trace, the probability distribution of matrices can be written $\rho_M(d, b)$. What is the region in the (b, d) plane corresponding to the range of eigenvalue splittings $(\lambda, \lambda + \Delta)$? If ρ_M is continuous and finite at $d = b = 0$, argue that the probability density $\rho(\lambda)$ of finding an eigenvalue splitting near $\lambda = 0$ vanishes (level repulsion).* (Hint: Both d and b must vanish to make $\lambda = 0$. Go to polar coordinates, with λ the radius.)

(c) *Calculate analytically the standard deviation of a diagonal and an off-diagonal element of the GOE ensemble (made by symmetrizing Gaussian random matrices with $\sigma = 1$).* You may want to check your answer by plotting your predicted Gaussians over the histogram of H_{11} and H_{12} from your ensemble in part (a). *Calculate analytically the standard deviation of $d = (c-a)/2$ of the $N = 2$ GOE ensemble of part (b), and show that it equals the standard deviation of b.*

(d) *Calculate a formula for the probability distribution of eigenvalue spacings for the $N = 2$ GOE, by integrating over the probability density $\rho_M(d, b)$.* (Hint: Polar coordinates again.)

If you rescale the eigenvalue splitting distribution you found in part (d) to make the mean splitting equal to one, you should find the distribution

$$\rho_{\text{Wigner}}(s) = \frac{\pi s}{2} \mathrm{e}^{-\pi s^2/4}. \tag{4}$$

This is called the *Wigner surmise*; it is within 2% of the correct answer for larger matrices as well.[3]

(e) *Plot eqn 4 along with your $N = 2$ results from part (a). Plot the Wigner surmise formula against the plots for $N = 4$ and $N = 10$ as well.*

Does the distribution of eigenvalues depend in detail on our GOE ensemble? Or could it be *universal*, describing other ensembles of real symmetric matrices as well? Let us define a ± 1 ensemble of real symmetric matrices, by generating an $N \times N$ matrix whose elements are independent random variables, each ± 1 with equal probability.

(f) *Generate an ensemble of $M = 1000$ symmetric matrices filled with ± 1 with size $N = 2$, 4, and 10. Plot the eigenvalue distributions as in part (a). Are they universal (independent of the ensemble up to the mean spacing) for $N = 2$ and 4? Do they appear to be nearly universal[4] (the same as for the GOE in part (a)) for $N = 10$? Plot the Wigner surmise along with your histogram for $N = 10$.*

[3] The distribution for large matrices is known and universal, but is much more complicated to calculate.

[4] Note the spike at zero. There is a small probability that two rows or columns of our matrix of ± 1 will be the same, but this probability vanishes rapidly for large N.

The GOE ensemble has some nice statistical properties. The ensemble is invariant under orthogonal transformations:

$$H \to R^\top H R \qquad \text{with} \quad R^\top = R^{-1}. \tag{5}$$

(g) *Show that* $\mathrm{Tr}[H^\top H]$ *is the sum of the squares of all elements of* H*. Show that this trace is invariant under orthogonal coordinate transformations (that is,* $H \to R^\top H R$ *with* $R^\top = R^{-1}$*).* (Hint: Remember, or derive, the cyclic invariance of the trace: $\mathrm{Tr}[ABC] = \mathrm{Tr}[CAB]$.)

Note that this trace, for a symmetric matrix, is the sum of the squares of the diagonal elements plus *twice* the squares of the upper triangle of off-diagonal elements. That is convenient, because in our GOE ensemble the variance (squared standard deviation) of the off-diagonal elements is half that of the diagonal elements (part (c)).

(h) *Write the probability density* $\rho(H)$ *for finding GOE ensemble member* H *in terms of the trace formula in part (g). Argue, using your formula and the invariance from part (g), that the GOE ensemble is invariant under orthogonal transformations:* $\rho(R^\top H R) = \rho(H)$*.*

This is our first example of an *emergent symmetry*. Many different ensembles of symmetric matrices, as the size N goes to infinity, have eigenvalue and eigenvector distributions that are invariant under orthogonal transformations *even though the original matrix ensemble did not have this symmetry*. Similarly, rotational symmetry emerges in random walks on the square lattice as the number of steps N goes to infinity, and also emerges on long length scales for Ising models at their critical temperatures.