Problem Set 7: Resonances, Bell, Randomness, Overlap Catastrophes
Graduate Quantum I
Physics 6572

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Due Monday Nov. 26

Last correction at November 27, 2012, 4:17 pm

Reading

Sakurai and Napolitano, sections 3.10, 5.7, 5.9

Sethna, *Mössbauer, the X-ray Edge, and Macroscopic Quantum Effects*, half-done draft manuscript from years ago.

7.1 Sakurai and Napolitano, exercise 5.23, "A one dimensional harmonic oscillator ... spatially uniform *force* ..."

7.2 Sakurai and Napolitano, exercise 5.35, "Consider an atom made up ..."

7.3 **Molecular Rotations.** (Quantum) ③

In class, we estimated the frequency of atomic vibrations, by generating a simple model of an atom of mass AM_P in a harmonic potential whose length and energy scales were set by electron physics (a Bohr radius and a fraction of a Rydberg). In the end, we distilled the answer that atomic vibrations were lower in frequency than those of electrons by a factor $\sqrt{M_P/m_e}$, times constants of order one.

Here we consider the frequencies of molecular *rotations*.

(a) *By a similar argument, derive the dependence of molecular rotation energy splittings on the mass ratio* M_P/m_e.

(b) *Find some molecular rotation energy splittings in the literature. Are they in the range you expect from your estimates of part (a)?*

7.4 **Bell.**[1] (Quantum,Qbit) ③

Consider the following cooperative game played by Alice and Bob: Alice receives a bit x and Bob receives a bit y, with both bits uniformly random and independent. The players win if Alice outputs a bit a and Bob outputs a bit b, such that $(a+b = xy) mod 2$. They can agree on a strategy in advance of receiving x and y, but no subsequent communication between them is allowed.

(a) *Give a deterministic strategy by which Alice and Bob can win this game with 3/4 probability.*

[1] This exercise was developed by Paul Ginsparg, based on an example by Bell '64 with simplifications by Clauser, Horne, Shimony, & Holt ('69).

(b) *Show that no deterministic strategy lets them win with more than 3/4 probability. (Note that Alice has four possible deterministic strategies* $[0, 1, x, \sim x]$*, and Bob has four* $[0, 1, y, \sim y]$*, so theres a total of 16 possible joint deterministic strategies.)*

(c) *Show that no probabilistic strategy lets them win with more than 3/4 probability. (In a probabilistic strategy, Alice plays her possible strategies with some fixed probabilities* $p_0, p_1, p_x, p_{\sim x}$*, and similarly Bob plays his with probabilities* $q_0, q_1, q_y, q_{\sim y}$*.)*

The upper bound of <= 75% of the time that Alice and Bob can win this game provides, in modern terms, an instance of the Bell inequality, where their prior cooperation encompasses the use of any local hidden variable.

Let's see how they can beat this bound of 3/4, by measuring respective halves of an entangled state, thus quantum mechanically violating the Bell inequality.[2]

Suppose Alice and Bob share the entangled state $\frac{1}{\sqrt{2}}(|\uparrow\rangle_\ell|\uparrow\rangle_r + |\downarrow\rangle_\ell|\downarrow\rangle_r)$, with Alice holding the left Qbit and Bob holding the right Qbit. Suppose they use the following strategy: if $x = 1$, Alice applies the unitary matrix $R_{\pi/6} = \begin{pmatrix} \cos\frac{\pi}{6} & -\sin\frac{\pi}{6} \\ \sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{pmatrix}$ to her Qbit, otherwise doesn't, then measures in the standard basis and outputs the result as a. If $y = 1$, Bob applies the unitary matrix $R_{-\pi/6} = \begin{pmatrix} \cos\frac{\pi}{6} & \sin\frac{\pi}{6} \\ -\sin\frac{\pi}{6} & \cos\frac{\pi}{6} \end{pmatrix}$ to his Qbit, otherwise doesn't, then measures in the standard basis and outputs the result as b. (Note that if the Qbits were encoded in photon polarization states, this would be equivalent to Alice and Bob rotating measurement devices by $\pi/6$ in inverse directions before measuring.)

(d) *Using this strategy: (i) Show that if* $x = y = 0$*, then Alice and Bob win the game with probability 1.*
(ii) Show that if $x = 1$ *and* $y = 0$ *(or vice versa), then Alice and Bob win with probability 3/4.*
(iii) Show that if $x = y = 1$*, then Alice and Bob win with probability 3/4.*
(iv) Combining parts (i)–(iii), conclude that Alice and Bob win with greater overall probability than would be possible in a classical universe.

This proves an instance of the CHSH/Bell Inequality, establishing that "spooky action at a distance" cannot be removed from quantum mechanics. Alice and Bob's ability to win the above game more than 3/4 of the time using quantum entanglement was experimentally confirmed in the 1980s (A. Aspect et al.).[3]

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[2] There's another version for GHZ state, where three people have to get a+b+c mod 2 = x or y or z. Again one can achieve only 75% success classically, but they can win *every* time sharing the right quantum state

[3] Ordinarily, an illustration of these inequalities would appear in the physics literature not as a game but as a hypothetical experiment. The game formulation is more natural for computer scientists, who like to think about different parties optimizing their performance in various abstract settings. As mentioned, for physicists the notion of a classical strategy is the notion of a hidden variable theory, and the quantum strategy involves setting up an experiment whose statistical results could not be predicted by a hidden variable theory.

(e) *(Bonus) Consider a slightly different strategy, in which before measuring her half of the entangled pair Alice does nothing or applies* $R_{\pi/4}$*, according to whether* x *is 0 or 1, and Bob applies* $R_{\pi/8}$ *or* $R_{-\pi/8}$*, according to whether* y *is 0 or 1. Show that this strategy does even better than the one analyzed in a–c, with an overall probability of winning equal to* $\cos^2 \pi/8 = (1 + \sqrt{1/2})/2 \approx .854$.
(Extra bonus) Show this latter strategy is optimal within the general class of strategies in which before measuring Alice applies R_{α_0} *or* R_{α_1}*, according to whether* x *is 0 or 1, and Bob applies* R_{β_0} *or* R_{β_1}*, according to whether* y *is 0 or 1.*

This will demonstrate that no local hidden variable theory can reproduce all predictions of quantum mechanics for entangled states of two particles.

7.5 **Random matrix theory.**[4] (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

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

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

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

(a) *Generate an ensemble with* $M = 1000$ *or so GOE matrices of size* $N = 2$, 4, *and* 10. *(More is nice.) 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*[5] $N/2$. *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 $M = 1000$.)

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

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

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

This is called the *Wigner surmise*; it is within 2% of the correct answer for larger matrices as well.[6]

(e) *Plot eqn 2 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.*

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

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

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*[7] *(the same as for the GOE in part (a)) for* $N = 10$*? Plot the Wigner surmise along with your histogram for* $N = 10$.

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

$$H \to R^\top H R \qquad \text{with} \;\; R^\top = R^{-1}. \tag{3}$$

(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.

7.6 **Quantum dissipation from phonons.** (Quantum) ②

Electrons cause overlap catastrophes (X-ray edge effects, the Kondo problem, macroscopic quantum tunneling); a quantum transition of a subsystem coupled to an electron bath ordinarily must emit an infinite number of electron-hole excitations because the bath states before and after the transition have zero overlap. This is often called an *infrared* catastrophe (because it is low-energy electrons and holes that cause the zero

[7] 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.

overlap), or an *orthogonality* catastrophe (even though the two bath states aren't just orthogonal, they are in different Hilbert spaces). Phonons typically do not produce overlap catastrophes (Debye–Waller, Frank–Condon, Mössbauer). This difference is usually attributed to the fact that there are many more low-energy electron-hole pairs (a constant density of states) than there are low-energy phonons ($\omega_k \sim ck$, where c is the speed of sound and the wave-vector density goes as $(V/2\pi)^3 \mathrm{d}^3 k$).

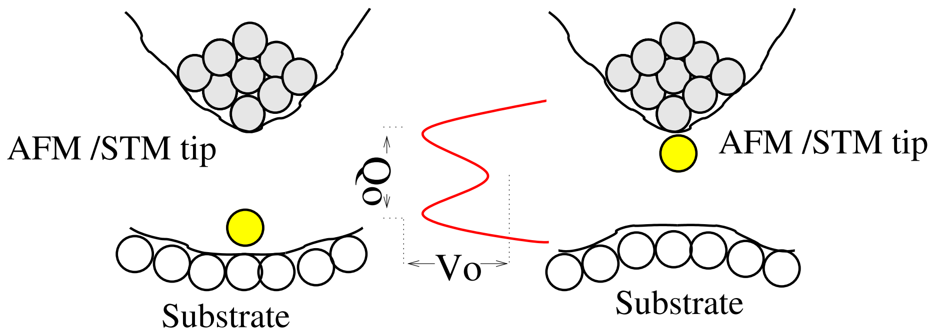

Fig. 1 Atomic tunneling from a tip. Any *internal* transition among the atoms in an insulator can only exert a force impulse (if it emits momentum, say into an emitted photon), or a force dipole (if the atomic configuration rearranges); these lead to non-zero phonon overlap integrals only partially suppressing the transition. But a quantum transition that changes the net force between two macroscopic objects (here a surface and a STM tip) can lead to a change in the net force (a force monopole). We ignore here the surface, modeling the force as exerted directly into the center of an insulating elastic medium.[8] See "Atomic Tunneling from a STM/AFM Tip: Dissipative Quantum Effects from Phonons" Ard A. Louis and James P. Sethna, *Phys. Rev. Lett.* **74**, 1363 (1995), and "Dissipative tunneling and orthogonality catastrophe in molecular transistors", S. Braig and K. Flensberg, *Phys. Rev. B* **70**, 085317 (2004).

However, the coupling strength to the low energy phonons has to be considered as well. Consider a small system undergoing a quantum transition which exerts a net force at $x = 0$ onto an insulating crystal:

$$\mathcal{H} = \sum_k p_k^2/2m + 1/2\, m\omega_k^2 q_k^2 + F \cdot u_0. \tag{4}$$

Let us imagine a kind of scalar elasticity, to avoid dealing with the three phonon branches (two transverse and one longitudinal); we thus naively write the displacement of the atom at lattice site x_n as $u_n = (1/\sqrt{N}) \sum_k q_k \exp(-\mathrm{i}kx_n)$ (with N the number of atoms), so $q_k = (1/\sqrt{N}) \sum_n u_n \exp(\mathrm{i}kx_n)$.

Substituting for u_0 in the Hamiltonian and completing the square, find the displacement Δ_k of each harmonic oscillator. (Physically, the force F adds a small linear term to the phonon mode with wavevector k, whose minimum becomes displaced by some amount Δ_k.) Let $|F\rangle$ be the ground state of the harmonic oscillators under the force

F. Write the formula for the likelihood $\langle F|0\rangle$ *that the phonons will all end in their ground states, as a product over* k *of the phonon overlap integral* $\exp(-\Delta_k^2/8\sigma_k^2)$ *(with* $\sigma_k = \sqrt{\hbar/2m\omega_k}$ *the zero-point motion in that mode). Converting the product to the exponential of a sum, and the sum to an integral* $\sum_k \sim (V/(2\pi)^3 \int \mathrm{d}k$*, do we observe an overlap catastrophe?*

Note that you've calculated the probability of a zero-phonon transition – the likelihood that the quantum transition can happen without emitting any phonons is zero. But the same argument shows that there is zero probability of emitting one phonon, or any finite number of phonons. The only allowed transitions emit an infinite number of low-energy phonons. The initial and final ground states are in 'different Hilbert spaces' – no finite number of excitations can connect them.