Problem Set 3: Entanglement & Free Particles
Graduate Quantum I
Physics 6572

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Due Fri Sept. 12 (turn in Wednesday or in class homework box)
Last correction at August 27, 2014, 9:30 am

NOTE: No class Friday September 12. Attend the Henley symposium!

Potentially useful reading

Sakurai and Napolitano, section 1.4 (Uncertainty)
Weinberg sections 3.3 (Uncertainty), 12.1 (Entanglement)
Sethna, "Entropy, Order Parameters, and Complexity" appendix A (Evolving Schrödinger)
Schumacher & Westmoreland sections 6.1, 6.2, 6.4 (Entanglement), 6.5, 6.6, 6.7 (GHZ), Appendix B (Evolving Schrödinger)

3.1 **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 2.4(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 2.4(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?*

3.2 **Coherent And Incoherent Bits.** (Schumacher and Westmoreland Problem 2.8) ②

Two boxes each produce a stream of qubits. Box A produces the qubits all in the state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Box B randomly produces qubits in states $|0\rangle$ and $|1\rangle$, each with probability 1/2. We have one of the boxes, but it is unmarked and so we do not know which kind it is. Describe an experiment on the qubits that can tell the difference between box A and box B. Can you reliably tell the difference between the boxes by examining only one of the qubits?

3.3 **GHZ States.** (Schumacher and Westmoreland Problem 6.6) ③

Consider the GHZ state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0,0,0\rangle - |1,1,1\rangle)$, where Alice, Bob and Charles possess the first, second and third bits respectively.

(a) *Suppose that Alice makes a Z measurement on her qubit. Show that the qubits of Bob and Charlie are in a product state, regardless of the measurement result.*

(b) *Suppose Alice makes an X measurement on her qubit. Show that Bob and Charlie's qubits end up in an entangled state, regardless of the measurement result.*

3.4 **Anti-Singlets.** (Schumacher and Westmoreland Problem 6.8) ③

Section 6.6 of Schumacher and Westmoreland showed that if two qubits are in the singlet state $\langle S| = \frac{1}{\sqrt{2}}(\langle\uparrow|_l\langle\downarrow|_r - \langle\downarrow|_l\langle\uparrow|_r)$, then measurements of parallel spin components (in the XZ plane) always yield opposite results.

(a) *Show that this is also true for Y measurements on* $|S\rangle$.

(b) *Does there exist an "anti-singlet" state of two qubits, for which measurements of parallel spin components always yield identical results? If so, write down the state vector. If not, give a proof that no state, product or entangled, can do this.*

3.5 **Momentum commutators, magnetism, and Landau levels.** (Sakurai Problem 2.37) ③

An electron moves in the presence of a uniform magnetic field in the z-direction ($\mathbf{B} = B\hat{\mathbf{z}}$)

(a) *Evaluate* $[\Pi_x, \Pi_y]$, *where* $\Pi_x = p_x - \frac{eA_x}{c}$ *and* $\Pi_y = p_y - \frac{eA_y}{c}$

(b) *By comparing the Hamiltonian and the commutation relation obtained in (a) with those of the one-dimensional oscillator problem, show how we can immediately write the energy eigenvalues as*

$$E_{k,n} = \frac{\hbar^2 k^2}{2m} + \left(\frac{|eB|\hbar}{mc}\right)\left(n + \frac{1}{2}\right),$$

where $\hbar k$ *is the the continuous eigenvalues of the* p_z *operator and* n *is a non-negative integer including zero.*

3.6 **Evolving Schrödinger: Free particles and uncertainty.** (Computation) ③

Several of our computational exercises will involve solving the time-dependent Schrödinger equation for one-dimensional quantum systems. In this first of these exercises, we shall evolve the free particle Hamiltonian

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\psi = H_{\mathrm{kin}}\psi \\ \psi(x,t) &= U(t)\psi(0) = \mathrm{e}^{-\mathrm{i}H_{\mathrm{kin}}t/\hbar}\psi(x,0) \end{aligned} \tag{1}$$

In a later exercise, we shall solve for the behavior of a hydrogenic harmonic oscillator with angular frequency $\omega = 10^{12}$ radians/sec. We'll use the ground state of this harmonic oscillator as our initial condition for the free-particle evolution:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-m\omega x^2/2\hbar} = \left(\frac{1}{2\pi a_0^2}\right)^{1/4} \mathrm{e}^{-x^2/4a_0^2}. \tag{2}$$

Here $a_0 = \sqrt{\hbar/2m\omega}$ is the root-mean-square width of the Gaussian probability distribution $|\psi(x)|^2$.

With no potential energy, we can solve for the motion of a free particle, $\widetilde{\psi}(k,t) = U_{\mathrm{kin}}(t)\psi(k,t=0)$ using Fourier transforms.

$$\widetilde{\psi}(k,t) = \mathrm{e}^{-\mathrm{i}(\hbar k^2/2m)t}\widetilde{\psi}(k,t=0) \tag{3}$$

$$\widetilde{\psi}(x,t) = IFFT[\mathrm{e}^{-\mathrm{i}(\hbar k^2/2m)t} FFT[\widetilde{\psi}(x,t=0)]] \tag{4}$$

where FFT takes a Fourier transform of the wavepacket, and IFFT takes an inverse Fourier transform. (FFT stands for Fast Fourier Transform.)

Let's numerically solve for the evolution of $\psi_0(x)$ from eqn 2. We'll evaluate it at a discrete set of $N_p = 200$ points spanning a distance $L = 80a_0$. With $\mathrm{d}x = L/N_p$, the points will be at $-L/2, L/2 + \mathrm{d}x, \ldots, L/2 - \mathrm{d}x$. In CGS units, the hydrogen mass is about the proton mass 1.672610^{-24} gm, $\hbar = 1.0545710^{-27}$ erg sec, and we decided $\omega = 10^{12}$ radians/sec.

(a) *Define ψ_0 on this grid. Plot your $|\psi_0|^2$, and check that it roughly has width a_0.*

The Fast Fourier Transform of ψ returns $\widetilde{\psi}(k)$ evaluated at points

$$k = (0, \mathrm{d}k, 2\mathrm{d}k, \ldots, -2\mathrm{d}k, -\mathrm{d}k), \tag{5}$$

with $\mathrm{d}k = 2\pi/L$. (These correspond to the plane waves with period L; FFTs assume periodic boundary conditions.) The maximum value $k_{\mathrm{max}} = \pi/\mathrm{d}x$ happens in the *center* of the FFT. To do our time evolution, we need to define an array k^2 evaluated at these points, which should rise quadratically, come to a cusp, and then fall back to zero.

(b) *Define k^2 on this grid. Plot it.*

Now we can evolve $\psi(x,t) = U_{\mathrm{kin}}(t)\psi_0(x)$.

(c) *Create a routine that calculates $\psi(x,t)$ using eqn 4. Plot the real and imaginary parts of $\psi(x,t)$ at $t = P/4$, P, and $2P$ on separate plots, where $P = 2\pi/\omega$ is the period of the harmonic oscillator in the later exercise. What happens to the width of the wave packet?*

The Heisenberg uncertainty principle tells us that $\Delta x \Delta p \geq \hbar/2$. The Gaussian wavepacket we use is the form that minimizes this inequality, so we expect the packet width to grow like vt with v given by the momentum uncertainty $v \sim \Delta p/m$

(d) *Give the formula for v for our packet. Calculate $\Delta x = \sqrt{\langle x^2 \rangle}$ as a function of time, for points $0 \leq t \leq 2P$. Plot Δx versus time and vt versus time on the same plot. Why do they not agree at short times?*

3.7 **Entangled Spins.** (Spins) ③

In class, we studied the entanglement of the singlet spin state $|\mathcal{S}\rangle = (1/\sqrt{2})(|\uparrow\rangle_\ell|\downarrow\rangle_r - |\downarrow\rangle_\ell|\uparrow\rangle_r)$ of electrons of a diatomic molecule as the atoms L and R are separated;[1] the spins on the two atoms are in opposite directions, but the system is in a superposition of the two choices. Here we discuss another such superposition, but with a different relative phase for the two choices:

$$|\chi\rangle = (1/\sqrt{2})(|\uparrow\rangle_\ell|\downarrow\rangle_r + |\downarrow\rangle_\ell|\uparrow\rangle_r) \tag{6}$$

You should know from angular momentum addition rules that the space of product wavefunctions of two spin $\frac{1}{2}$ states can be decomposed into a spin 1 and a spin 0 piece: $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$. So there are two orthogonal eigenstates of S_z with eigenvalue zero: one of total spin zero and one of total spin one.

(a) **Total spin.** *Which state is which?* (If you don't know from previous work, calculate!) *Why do we call $|\mathcal{S}\rangle$ a singlet?*

Now, is the spin wavefunction compatible with what we know about electron wavefunctions?

(b) **Symmetry.** *When the two spins are exchanged, how does $|\chi\rangle$ change? If the total wavefunction $\Psi(x_L, s_L, x_R, s_L)$ is a product of this spin wavefunction $\chi(s_L, s_R)$ and and a two-particle spatial wavefunction $\psi(x_L, x_R)$, what symmetry must ψ have under interchange of electrons?*

We noted in class that two other spin-1 product states, $|\uparrow\rangle_\ell|\uparrow\rangle_r$ and $|\downarrow\rangle_\ell|\downarrow\rangle_r$ do not form entangled states when L and R separate. Is $|\chi\rangle$ like these spin-1 states, or is it entangled like $|\mathcal{S}\rangle$ is?

(c) **Entanglement.** *Give the Schmidt decomposition of $|\chi\rangle$. What are the singular values? What is the entanglement entropy?* (Hint: The steps should be very familiar from class.)

(d) **Singular Value Decomposition (SVD).** *Let M be the matrix which gives $|\chi\rangle$ as a product of left and right spin states:*

$$|\chi\rangle = \left(\Uparrow\rangle_\ell \; \Downarrow\rangle_\ell \right) M \begin{pmatrix} \Uparrow\rangle_r \\ \Downarrow\rangle_r \end{pmatrix}. \tag{7}$$

What is M? Give an explicit singular value decomposition[2] $M = U\Sigma V^T$ of the matrix M. Explain how the SVD gives us the Schmidt decomposition of part (c).

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[1] We assumed that, when separated, one electron is localized basically on each of the two atoms, and the spin kets are labeled based on the primary locale of the corresponding spatial wavefunction for that electron.

[2] Remember that the SVD guarantees that U and V have orthonormal columns, and Σ is a diagonal matrix whose diagonal elements σ_i are all positive and decreasing (so $\sigma_i \geq \sigma_{i+1} \geq 0$). There is some flexibility in the singular vectors (i.e., matched pairs can both have their signs changed), but the singular values are unique and hence a property of the matrix.