THE UNIVERSITY OF BRITISH COLUMBIA

Physics 210 Assignment # 9: MATRIX MADNESS!

Tue. 16 Nov. 2010 — finish by Tue. 23 Nov.

Since the course descriptions headlines MatLab, let's do something truly "computational" with it. (I will describe the exercises in terms of MatLab, but you are welcome to use `octave` or `python` instead, as they will both do everything required for this Assignment at least as well as MatLab does. Just pick your favorite!)

As usual, create your `/home2/phys210/$USER/a09/` directory to store your work in.

1. MATLAB WARMUP: Remember the Fibonacci numbers from earlier Assignments? In a file `fibmat.m`, write a MatLab function to generate the Fibonacci numbers F_n and *plot* the resulting F_n as a function of n (up to at least $n = 10$)[1] so it will be easy to check your work. Store your plot in `/home2/phys210/$USER/a09/fib.pdf` (using *ImageMagick*'s `convert` if necessary).

2. PAULI MATRICES: The most important matrices in Physics (so say I) are the Pauli spin matrices, described accurately in the *WikipediA*[2] as "a set of 2×2 complex Hermitian and unitary matrices..."

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \; \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \; \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (1)$$

which can represent (among other things) the three components ($\sigma_x \equiv \sigma_1$, $\sigma_y \equiv \sigma_2$ and $\sigma_z \equiv \sigma_3$) of the vector **spin operator** $\vec{\sigma}$ for a spin-$\frac{1}{2}$ particle.[3] Well, MatLab claims to be a "Matrix Laboratory", so it should be an ideal platform for verifying the essential properties of the Pauli matrices.[4] *Do so*, for the list of properties listed on `http://en.wikipedia.org/wiki/Pauli_matrices` down to the beginning of the subject heading labelled "$SU(2)$". Make sure you understand the meaning of all these properties thoroughly.[5]

In this notation, the spin state of a spin-$\frac{1}{2}$ particle is represented by a 2-component column vector, like

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (2)$$

for "spin up" and "spin down" (along the $\hat{z}$ axis) respectively. Verify that operating on these column vectors from the left with the Pauli matrix σ_z yields $+|\uparrow\rangle$ and $-|\downarrow\rangle$, respectively.[6]

Construct a column vector $|\rightarrow\rangle$ with the property that $\sigma_x|\rightarrow\rangle = +|\rightarrow\rangle$ (so that $|\rightarrow\rangle$ represents a spin-$\frac{1}{2}$ particle with its spin in the $+\hat{x}$ direction).

Similarly, construct a column vector $|\otimes\rangle$ with the property that $\sigma_y|\otimes\rangle = +|\otimes\rangle$ (so that $|\otimes\rangle$ represents a spin-$\frac{1}{2}$ particle with its spin in the $+\hat{y}$ direction).

3. TWO SPIN-$\frac{1}{2}$ PARTICLES: Suppose you have *two* spin-$\frac{1}{2}$ particles, such as a proton (p) and an electron (e), whose magnetic moments $\vec{\mu}_p = \mu_p \, \vec{\sigma}_p$ and $\vec{\mu}_e = -\mu_e \, \vec{\sigma}_e$ interact with an external magnetic field $\vec{B}$, each contributing its *Zeeman energy* $E_Z = -\vec{\mu} \cdot \vec{B}$. Then the *Zeeman hamiltonian operator* is

$$\mathcal{H}_Z = -\mu_p \, \vec{\sigma}_p \cdot \vec{B} + \mu_e \, \vec{\sigma}_e \cdot \vec{B}. \quad (3)$$

Again picking the $\hat{z}$ direction as the quantization axis, we have *four* possible fully-specified quantum states:

$$|\Uparrow\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad |\Uparrow\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$|\Downarrow\uparrow\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad |\Downarrow\downarrow\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \quad (4)$$

where the $\Updownarrow$ and $\updownarrow$ symbols designate "spin up/down" (along the $\hat{z}$ axis) for the electron and the proton, respectively.

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[1] If you go to n much larger than 10, it might be wise to plot $\log F_n$ *vs.* n.

[2] You can *Google* them, or go directly to `http://en.wikipedia.org/wiki/Pauli_matrices` or `http://mathworld.wolfram.com/PauliMatrices.html` to get a nice compact introduction to their mathematical properties. Be sure you understand what "Hermitian" and "unitary" mean.

[3] Actually, the Pauli matrices can be used to describe the quantum mechanics of *any two-state system*, which makes them useful not only in elementary particle physics but also in a wide variety of *quantum computing* topics.

[4] I don't find MatLab to be as great as it claims, since I have not found a compact, elegant way to express the three Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$ as a *vector* $\vec{\sigma}$ of matrices in MatLab, even though that is a "natural" description in Physics. This *is* possible with `python`; Google "`NumPy` for `Matlab` Users".

[5] You'll thank me later!

[6] Thus $|\uparrow\rangle$ and $|\downarrow\rangle$ are the *eigenvectors* of σ_z: operating on them with σ_z is the same as multiplying them by a number which is their *eigenvalue* with respect to σ_z. In the language of spin orientation, the eigenvalue is the projection of the particle's spin along the $\vec{z}$ direction). This follows from the fact that σ_z is *diagonal*.

In this basis, verify that the 4×4 matrix representations of the electron and proton spin operators are

$$\sigma_{e_1} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} ; \quad \sigma_{p_1} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad (5)$$

$$\sigma_{e_2} = \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} ; \quad \sigma_{p_2} = \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix}$$

$$\sigma_{e_3} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} ; \quad \sigma_{p_3} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

Given this information, write down the matrix representation of the full Zeeman hamiltonian for these two spins in an arbitrary magnetic field $\vec{B} = B_x \hat{x} + B_y \hat{y} + B_z \hat{z}$. Express your result in terms of μ_p, μ_e and the three components of $\vec{B}$.

4. THE CONTACT INTERACTION: Suppose your two spin-$\frac{1}{2}$ particles (*e.g.* the proton and the electron in a hydrogen atom) interact in a way that depends only on the scalar product of their spin vectors,[7]

$$\mathcal{H}_{\rm hf} = A\, \vec{\sigma}_p \cdot \vec{\sigma}_e = A(\sigma_{p_1}\sigma_{e_1} + \sigma_{p_2}\sigma_{e_2} + \sigma_{p_3}\sigma_{e_3}) , \qquad (6)$$

where $\mathcal{H}_{\rm hf}$ is the *Heisenberg hamiltonian* operator and A is the strength of the interaction, in energy units. For simplicity, set $A = 1$ (*i.e.* measure all energies as multiples of A) in this part.

Express the Heisenberg spin hamiltonian (6) as a *matrix* in the 4-state basis (4) defined above, and show that it is *not diagonal*. Using MatLab, *diagonalize it* and *describe the new basis* in which it is diagonal.[8]

[7] Such an interaction is known as a contact interaction or a hyperfine interaction or a Heisenberg spin-spin interaction.

[8] If you need help with this, just ask!

5. BREIT-RABI DIAGRAM: [EXTRA CREDIT] We are now ready to solve the general problem of the spin hamiltonian (which governs everything the spins do!) of a hydrogen atom in an s state with orbital angular momentum $\ell = 0$.[9] The *Breit-Rabi hamiltonian* is

$$\mathcal{H}_{\rm BR} = \mathcal{H}_{\rm hf} + \mathcal{H}_Z$$
$$= A\, \vec{\sigma}_p \cdot \vec{\sigma}_e - \mu_p\, \vec{\sigma}_p \cdot \vec{B} + \mu_e\, \vec{\sigma}_e \cdot \vec{B}. \qquad (7)$$

Express this hamiltonian in matrix form for the 4-state basis (4) and (using MatLab) *diagonalize it* for some particular choice of applied magnetic field, let's say $\vec{B} = (0.1 \text{ T})\hat{z}$. Once you have accomplished this, you can repeat the diagonalization for a succession of different values of $|\vec{B}| = B_z$ and plot the four energy eigenvalues as a function of field to get the famous *Breit-Rabi diagram* for hydrogen:

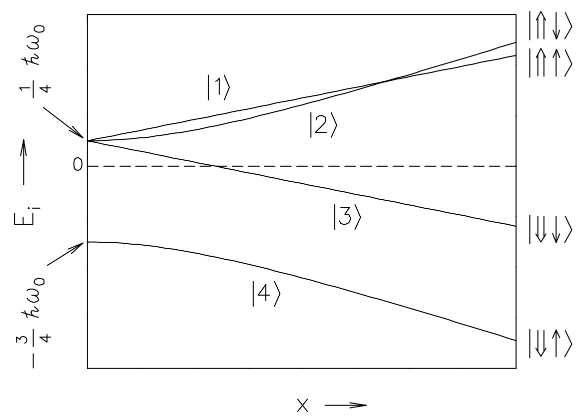

Figure 1 : *Breit-Rabi diagram* showing the energy levels of a system of two spin-1/2 particles of opposite sign and different magnetic moments (*e.g.* the hydrogen atom) as functions of the *reduced field* $x \equiv B/B_0$ where B_0 (504.4 Oe for H in vacuum) is a characteristic *hyperfine field*. For the purpose of illustration, unphysical values of moments and coupling constants have been used.

The actual *hyperfine frequency* $\nu_0 \equiv \omega_0/2\pi \equiv A/h$ (where h is Planck's constant) has the value 1.42040575 GHz for hydrogen in vacuum. In consistent units, $\mu_e/h = -28.024953$ GHz/T and $\mu_p/h = 0.042577482$ GHz/T.

In zero field the three *triplet* ($J = 1$) eigenstates $|1\rangle$, $|2\rangle$ and $|3\rangle$ are degenerate and the *singlet* ($J = 0$) ground state $|4\rangle$ is $\hbar\omega_0$ lower in energy.

At high reduced field ($x \to \infty$) the eigenstates are $|1\rangle \to |\Uparrow\uparrow\rangle$, $|2\rangle \to |\Uparrow\downarrow\rangle$, $|3\rangle \to |\Downarrow\downarrow\rangle$ and $|4\rangle \to |\Downarrow\uparrow\rangle$. That is, the original basis!

[9] Actually there are $\ell \neq 0$ states mixed into the "1s" state of a hydrogen atom if the two spins are parallel; but this is a very small effect.