Teaching advanced physics in the age of computers

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Workshop on the Teaching of Computational Physics
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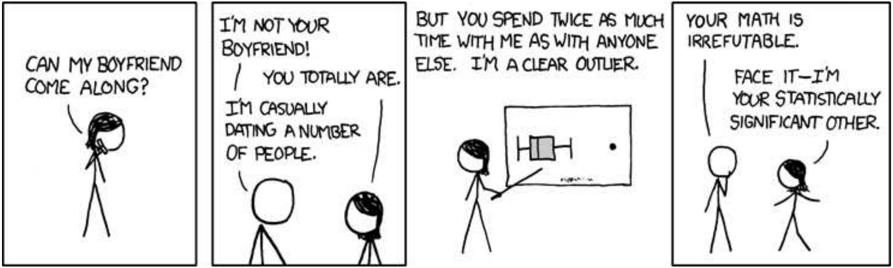
Outline

1. Ubiquitous computing
2. An experiment in teaching Quantum Mechanics
3. Notes from the course
4. Further questions

Insidious computing



How fast?

- A typical high end desktop today could be a Core 2 Duo with a clock speed of about 3 GHz. This is faster than a Cray YMP, which was the supercomputing workhorse of the early 1990's.
- The oldest motherboard for which we can still get replacements is a Intel 845 with a clock speed of 2.4 GHz. This is as fast as a Cray XMP, which was the supercomputer of choice in the mid-1980's. The Cray XMP was used for code breaking and computations of hydrodynamics needed for the design of nuclear devices.
- These desktop supercomputers are used mainly to check mails.

How many?

- Almost 250 million Indians carry a cell phone. Each modern cell phone is capable of solving problems from Jackson in a jiffy (and displaying the results as a colour plot). Students have better cell phones than their teachers.
- By now many university departments have multiple PC's and workstations. College departments typically have few. How can one make the best use of these? **Some discussion needed on access: safe department-wide login vs grid gateway to mobile devices.**
- For Rs. 30,000 one can buy an entry level machine which is faster than a YMP. With various kinds of grants it is possible for departments to build up very good computing labs to cater to classes of about 100 students. **Some discussion needed on finance and technique?**
- Providing access points is the main problem: typically limited by keyboard and screen. Gateway to mobile devices would solve this problem.

Ubiquitous computing: a day in your life

- You use e-mail more often now than five years ago, and will use it more often in the future than you use it now. Web access on mobile devices is already becoming cheaper.
- You still write and use compiled programs in efficient languages like C or FORTRAN for the most compute intensive parts of your work.
- You probably present lectures in electronic form more often than in the past. You use LaTeX, ppt or openoffice to write, and gnuplot, xfig, perhaps Mathematica to plot. You probably prepare small computations using paper and pencil, some calculator, and perhaps Mathematica (or equivalent).
- Your leisure time probably involves more "computing devices" today than in the 90's: set-top boxes, MP3 for music, Photoshop, gimp or Picasa for your photos, YouTube and movies on the computer, Google, Wikipedia, electronic magazines for general reading, Skype, Twitter and blogs to communicate with friends and family.

Ubiquitous computing: how has it changed science?

- Computations are an intrinsic part of the life of a theoretical physicist: every member of my department computes, either with compiled programs or interpreters like Mathematica. Most of these techniques are picked up in the course of work: as a result, the wheel is reinvented every day.
  - Large scale image processing has transformed astronomy.
  - Genomics and proteomics are impossible without supercomputing.
  - Field theory is now, in a very real sense, lattice gauge theory.
  - Any imaging device is now half software.
- Every little lab has a DAQ: usually a commercial product called LabView, which (among other things) allows you to write a C program using a graphical interface in which you drag and drop boxes.
- Any lab which builds instruments now needs CAD/CAM software like SolidWorks to design them. The designs are often transferred to NC machines for fabrication.

Has ubiquitous computing entered coursework?

- Object-oriented programming is now taught in schools. By class IX some students are programming in Java or C++.
- In many universities numerical analysis is still the only course on computational aspects of physics that is offered.
- In some universities a computational physics course is now offered in addition to the numerical analysis course.
- The actual content of under/graduate courses still contains exactly the same material that was used in the 70's, based on courses developed in the 30's. In many cases, we still use the classic books: Jenkins and White or Born and Wolf for optics, Jackson (or something closely related) for electrodynamics, Schiff (and functional equivalents including Shankar) for Quantum Mechanics.
- Ubiquitous computing does not find a place in physics teaching as yet: except for (as yet) isolated experiments.

Where can we introduce ubiquitous computing?

EVERYWHERE

Elementary calculus, variational calculus, solutions of differential equations, functional bases, combinatorial enumeration, probability and statistics, complex variables, linear algebra, group theory...

The reason for this ubiquity of computational methods in physics is that our teaching is geared to the practical problem of getting numbers from theories.

The basic technique

Everything is concrete

Use computation to make concrete any abstract idea you want to introduce. This frees you to use a high level of "abstraction" in your lectures. No idea is abstract any more, every concept becomes grounded in practice.

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Everything is solvable

To implement this procedure you can introduce the idea of "top-down problem solving" (Polya: How to solve it). Given a problem, keep breaking it down into component pieces until all the pieces you have are problems which have been solved before. In other words: think before you write.

Outline

Basic observations

- One can assume that students are familiar with ordinary three-vectors and basic notions of transformation of bases. I assumed that students know vector addition, dot products and cross products, and would recall, with a little prompting, how to rotate vectors.
- The structure of quantum mechanics which one wants to teach is unchanged from Dirac's book. This is the conceptual understanding which any student should have at the end of the course.
- Quantum mechanics (Hilbert space as opposed to Fock space) is essentially used to solve few-body systems: for example, atomic physics or nuclear physics. The techniques used in these research problems are matrix diagonalization. No one actually solves differential equations any more.
- The course can be re-oriented so that students learn how write down matrices corresponding to a given quantum-mechanics problem. They should learn about functional bases, approximations of functions, and a large number of techniques for dealing with linear systems.

Course home page: http://theory.tifr.res.in/~sgupta/courses/qm2008/

Two-state systems

- The Feynman Lectures popularized the use of two-state systems as a pedagogical tool. This tool is now widely used to introduce what Feynman called the "fundamental mystery of quantum mechanics".
- Modern textbooks (Baym in the 70's, Shankar in the 90's) took this further. They introduce the Dirac point of view (algebra of operators) using this example.
- It is possible to take this approach further. Introduce SU(2) as the most general symmetry group in this problem. Very concrete: learn the algebra by actually manipulating matrices.
- If computer algebra systems are available to students, then use the two state system as an opportunity to bias students towards top-down problem solving. This can be done even without exposure to computer algebra systems, but it is a little harder.

Collections of two-state systems

- After doing a single two-state system one can proceed to multi-particle systems. Introduce direct products of states. You are now ready to introduce Fock space if you wish, and the consequences of Bose and Fermi statistics.
- The real payoff comes in understanding angular momentum eigenstates. The notion of irreducible representations is introduced at this point, and all irreducible representations of SU(2) can be constructed algorithmically. Students can be asked to find these explicitly either by hand or by using a computer algebra system.
- The Clebsch-Gordan series and Clebsch-Gordan coefficients come out very naturally, since students have already been introduced to unitary transformations. In my experience, this demystifies this cluster of ideas by allowing students to work out a series of examples.

Outline

Building things up and breaking them down

We will build representations of larger j through direct products (also called tensor products) of lower representations. A direct product of two matrices N and M is the matrix

$$N \otimes M = \begin{pmatrix} n_{11}M & n_{12}M & n_{13}M & \cdots \\ n_{21}M & n_{22}M & n_{23}M & \cdots \\ n_{31}M & n_{32}M & n_{33}M & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix}.$$

The dimension of $N \otimes M$ is the product of the dimensions of each matrix. In general, $N \otimes M \neq M \otimes N$. Direct products of vectors follow from this definition. A direct sum of two matrices $N \oplus M$ is the block diagonal form

$$N \oplus M = \begin{pmatrix} N & 0 \\ 0 & M \end{pmatrix}.$$

The dimension of the direct sum is the sum of the dimensions of each matrix. We will now try to reduce direct products into direct sums.

Summing two momenta

If $|\mathbf{k}_1\rangle$ is the basis state of one particle and $|\mathbf{k}_2\rangle$ of another, then the direct product state $|\mathbf{k}_1;\mathbf{k}_2\rangle = |\mathbf{k}_1\rangle \otimes |\mathbf{k}_2\rangle$. The operator $\mathbf{p}_1 = \mathbf{p} \otimes 1$ acts only on the Hilbert state of the first particle, and the operator $\mathbf{p}_2 = 1 \times \mathbf{p}$ on the second. These operators commute since they act on different Hilbert spaces. The total momentum $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$.
Since all representations which we have built are one-dimensional, the direct product state is also one dimensional. One has

$$\mathbf{P}|\mathbf{k}_1;\mathbf{k}_2\rangle = (\mathbf{p}_1 + \mathbf{p}_2)\,|\mathbf{k}_1;\mathbf{k}_2\rangle = (\mathbf{k}_1 + \mathbf{k}_2)\,|\mathbf{k}_1;\mathbf{k}_2\rangle.$$

Therefore, the direct product state is the representation with momentum equal to the sum of the two momenta:

$$|\mathbf{k}_1\rangle \otimes |\mathbf{k}_2\rangle = |\mathbf{k}_1 + \mathbf{k}_2\rangle.$$

This is a fairly trivial example of direct product spaces. The case of direct products of angular momentum states is significantly different.

Summing two spins: counting dimensions

If $|j_1, m_1\rangle$ is the basis states of one particle, and $|j_2, m_2\rangle$ of another, then the direct product $|j_1, m_1\rangle \otimes |j_2, m_2\rangle = |j_1, m_1; j_2, m_2\rangle$. The operator $\mathbf{J}^{(1)} = \mathbf{j} \otimes 1$, *i.e.*, the operator for the first particle acts only on the Hilbert space of the first particle. Similarly, $\mathbf{J}^{(2)} = 1 \otimes \mathbf{j}$. All components of these two operators commute, since they act on different spaces. The total angular momentum of the system is $\mathbf{J} = \mathbf{J}^{(1)} + \mathbf{J}^{(2)}$. But

$$J^2|j_1, m_1; j_2, m_2\rangle \neq (j_1 + j_2)(j_1 + j_2 + 1)\hbar^2|j_1, m_1; j_2, m_2\rangle.$$

This is because the dimension of the direct product is $(2j_1 + 1)(2j_2 + 1)$ and this is not equal to $(2j_1 + 2j_2 + 1)$ unless either j_1 or j_2 (or both) is zero.

Example: The direct product of two $j = 1/2$ particles has dimension 4. This is either a $j = 3/2$ representation (which has dimension 4) or a direct sum of a $j = 0$ (dimension 1) and a $j = 1$ (dimension 3) representation. If the direct product can be reduced to a direct sum, then **all** components of $\mathbf{J}$ can be block diagonalized in this fashion.

Summing two spins: the spectrum of J_z

By the definition of the direct product, one has

$$J_z^1 = \begin{pmatrix} \hbar m_1 I & 0 & 0 \cdots & \\ 0 & \hbar(m_1-1)I & 0 & \cdots \\ 0 & 0 & \hbar(m_1-2)I & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix}, \qquad J_z^2 =?$$

J_z therefore remains diagonal. As a result, the quantum number M corresponding to the total J_z is the sum $m_1 + m_2$. In other words

$$J_z|j_1, m_1; j_2, m_2\rangle = (m_1 + m_2)\hbar|j_1, m_1; j_2, m_2\rangle.$$

Example: For the direct product of two $j = 1/2$ particles, the possible values of M are 1, -1, and 0 (twice). As a result, this direct product cannot be the representation $j = 3/2$. Therefore

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1.$$

A problem: summing two spins

Using the definition of the direct product for $|1/2, m_1; 1/2, m_2\rangle$, one has

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad J_+ = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad J_- = \frac{\hbar}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}.$$

Use this to find J^2 and check how to diagonalize it while keeping J_z diagonal. Using these results, show that

$$\begin{aligned} |1, 0\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\right\rangle + \left|\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\right\rangle\right), \\ |0, 0\rangle &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\right\rangle - \left|\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\right\rangle\right). \end{aligned}$$

Find the matrices corresponding to $\mathbf{J}$ in the $j = 1$ representation.

Summing two spins: the Clebsch-Gordan series

By the argument just presented, the states $|j, m; 1/2, m'\rangle$ can have total M ranging from $(j+1/2)$ to $-(j+1/2)$. The extreme eigenvalues are single, every other eigenvalue occurs twice. As a result,

$$j \otimes \frac{1}{2} = \left(j + \frac{1}{2}\right) \oplus \left(j - \frac{1}{2}\right).$$

By an inductive argument one can prove that the direct product states $|j_1, m_1; j_2, m_2\rangle$ can be decomposed as

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus (j_1 - j_2),$$

where each J occurs only once. The reduction of a direct product to direct sums of terms is called the **Clebsch-Gordan series**. In the CG series any value of $M = m_1 + m_2$, except the extremes, are degenerate. An unitary transformation among the various $|j_1, m_1; j_2, M - m_1\rangle$ is required to produce the angular momentum eigenstates $|J, M\rangle$. The unitary matrix is $|J, M\rangle\langle j_1, m_1; j_2, m_2|$. The matrix elements are called **Clebsch-Gordan coefficients**.

Examples of Clebsch-Gordan coefficients

1. The trivial CG coefficients are

$$\langle j_1 + j_2, j_1 + j_2 | j_1, j_1; j_2, j_2 \rangle = 1.$$

   One can in general write this as $\exp(i\psi)$ for some real ψ. The choice of ψ has to be compatible with the phase choices for the angular momentum eigenstates.

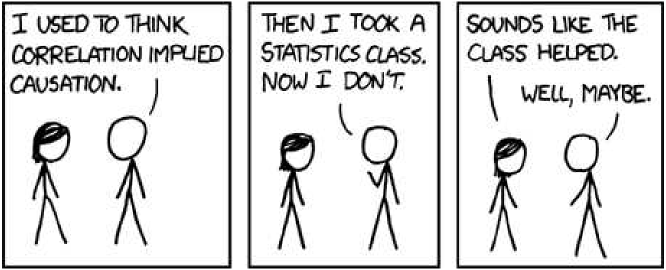
2. In the problem of the coupling of two spin 1/2 particles, the unitary transformation that rotates from the eigenbasis of the two uncoupled spins to the eigenbasis of the coupled spins is

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}.$$

   The CG coefficients $\langle 1, 1 | 1/2, 1/2; 1/2, 1/2 \rangle$, $\langle 1, -1 | 1/2, -1/2; 1/2, -1/2 \rangle$, $\langle 1, 0 | 1/2, m; 1/2, -m \rangle$, $\langle 0, 0 | 1/2, m; 1/2, -m \rangle$ can be read off this matrix.

Outline

Success


I USED TO THINK CORRELATION IMPLIED CAUSATION.
THEN I TOOK A STATISTICS CLASS. NOW I DON'T.
SOUNDS LIKE THE CLASS HELPED.
WELL, MAYBE.

Questions

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- How can research institutes and universities collaborate in the teaching of computational methods?