Teaching Density Functional Theory Through Experiential Learning

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Abstract. Today, quantum mechanical density functional theory is often the method of choice for performing accurate calculations on atomic, molecular and condensed matter systems. Here, I share some of my experiences in teaching the necessary basics of solid state physics, as well as the theory and practice of density functional theory, in a number of workshops held in developing countries over the past two decades. I discuss the advantages of supplementing the usual mathematically formal teaching methods, characteristic of graduate courses, with the use of visual imagery and analogies. I also describe a successful experiment we carried out, which resulted in a joint publication co-authored by 67 lecturers and students participating in a summer school.

1. Introduction
Today, quantum mechanical density functional theory is often the method of choice for performing accurate calculations on atomic, molecular and condensed matter systems. Such calculations provide data that can be used to interpret experiments, gain insight into structure-property relationships, and design novel materials. With recent rapid advances in computational power, it is now possible to perform such calculations on a desktop PC or laptop (or even, in some cases, on a mobile phone! [1]) With little need for infrastructure, this is an area of advanced research that can be easily embraced by students and scientists in the developing world. However, despite the widely prevalent view among many scientists that the teaching and practice of science is free of cultural influences, I (and, indeed, many others before me) have found that this is not true, and one has to take cultural factors into account even when teaching something that is as technical as physics.

2. Science, Culture, Teaching and Learning
The ways in which even subjects as seemingly “universal” as science or physics are taught, vary across cultures and countries: these differences are already manifested at the kindergarten and grade school level, where one observes either an instructionist or a constructionist method of teaching, with an emphasis placed either on information gathering or critical thinking.

In much of the developing world today, even science subjects are taught in a way that emphasizes rote memorization; this is certainly true of India, where I have spent a large part of my scientific career. There are two main possible reasons for this: one is that for millennia, the traditional way of teaching in India has involved learning texts “by heart”, the other is
that this is a colonial legacy – it did not suit colonial rulers to educate a native populace to think independently and critically; rather, their interests would be better served by having an “educated” cadre composed of individuals who would meekly carry out a prescribed set of instructions without stopping to analyze or critique them.

As a physics student in India in the 1970s and 1980s, I was often made to memorize physical laws and formulae (students who got a word wrong in the statement of a law were made to stand outside the class!); less emphasis was placed on problem solving or on understanding underlying physical principles.

It is clear that such training does not develop in students the critical skills necessary for a good scientist, and thus, efforts have to be made at the undergraduate and graduate level to help students make the transition from “knowledge” to “synthesis” [2, 3]. Among institutions in India that have won worldwide renown for their excellence in undergraduate science education are the Indian Institutes of Technology (IITs) and, more recently, the Indian Institutes of Science Education and Research (IISERs). However, these elite institutions can cater to only a small percentage of the student body across the country. Many students at smaller universities or colleges are desperate to learn, but lack mentors and/or access to resources.

3. Computational Physics and Density Functional Theory

I wish to argue that despite the well-known “digital divide” between the developed and developing countries, computational physics presents an ideal area where students of physics in developing countries can hope to do cutting-edge research.

This is because first, computational physics is relatively cheap. It is true that many computational physics groups worldwide use high-performance computing platforms, but with the increase in the speed and memory capacities of computers, and the accompanying decrease in the price of computers, today it is possible to tackle many interesting problems on a desktop PC or a laptop. Accordingly, this means that there are relatively low infrastructure requirements: electricity, water and air-conditioning can all be problems in developing countries, making it rather difficult to do high-quality experimental physics, for example.

As already mentioned in the Introduction, density functional theory (DFT) is, today, one of the most popular methods for treating condensed matter systems as well as other many-electron systems. The field has exploded in recent years, both due to the advances in computer technology, and due to methodological advances made in various aspects of how to map the many-electron Schrödinger equation “exactly” onto an equivalent system of one-particle equations. The 16 most-cited papers of all time in the Physical Review journals all deal with various aspects of DFT, and Walter Kohn was awarded the Nobel Prize in 1998 for his role in developing the field.

The number of lines in a typical DFT code is of the order of 100,000, and therefore few users of DFT write their own codes, and instead make use of standard packages. Today, there is a proliferation of DFT codes, some of which have to be purchased, and others which are freely downloadable. To mention the names of just a few DFT packages: QUANTUM ESPRESSO, VASP, Wien2K, Abinit, Siesta, FLEUR, CP2K, CPMD, etc. Many of these codes have user-friendly graphical user interfaces (GUIs). The apparent (misleading) ease of use of these interfaces and codes leads to a large number of students and scientists, all over the world, using them to perform calculations with little knowledge of what they are doing, using the code as a black box. Unfortunately, in such a situation, it is often possible, or even likely, that one will obtain completely meaningless results. There is therefore a great need for workshops where students can be trained to use such codes sensibly and appropriately.
4. QUANTUM ESPRESSO – The Distribution and Workshops

My experience of teaching DFT through experiential learning, especially in the developing world, has been gained through two main (and overlapping) platforms: the QUANTUM ESPRESSO schools, and ASESMA.

QUANTUM ESPRESSO [4, 5] is a distribution of codes that can perform standard DFT, density functional perturbation theory (DFPT) and time-dependent DFT calculations; it also comes equipped with many advanced features that have been developed in recent years. It is free and open-source, and comes equipped with the GNU public licence. An important activity of the QUANTUM ESPRESSO initiative is conducting training workshops, at both elementary and advanced levels. In part due to the close ties between the QUANTUM ESPRESSO developers and the Abdus Salam International Centre for Theoretical Physics in Trieste, there has been a special emphasis on conducting schools in developing countries. More than thirty such workshops have been conducted by the code developers; in addition, several workshops have also been conducted locally by various users of the codes.

The African Schools for Electronic Structure Methods and Applications (ASESMA) [6, 7] have been held biennially at various sites in Africa since 2010. They aim to train African students in electronic structure methods, following roughly the same pattern as that followed in the QUANTUM ESPRESSO schools.

While each training school or workshop may differ slightly in length and details, the typical duration is one to two weeks, with concepts and theory being covered in lectures in the mornings, and hands-on computer sessions in the afternoons, in which students apply the concepts learnt in the morning sessions. There is also often a project, in which students work in groups.

5. Teaching Through Visuals and Analogies

Since, in my experience, most students (and, often, especially those who have been trained in the developing world) are quite familiar with equations and mathematical formulations of problems, but have trouble translating this to conceptual knowledge, I find it helpful to make a lot of use of visuals and analogies while teaching the basics of solid state physics and DFT.

As an example of encouraging visual thinking, instead of just using the mathematical definition of a Bravais lattice:

\[ \mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \]  

I have students imagine that they are walking around on a sketched lattice, and picture the view they see – a Bravais lattice is one in which the view from each lattice point is the same (without turning around). Similarly, to understand the importance of the “plane-wave cutoff” used when performing DFT calculations in a plane-wave basis, I have them draw unit cells of various sizes, see how the Brillouin zones change accordingly in size, and thus the number of plane waves within the cutoff sphere, which in turn determines the size of the matrix that has to be diagonalized, and thus the computational time.

When it comes to analogies: my experience has been, the sillier the analogy, the more effective it is! One example that has proved popular is comparing the Kohn-Sham approach [8] of mapping the many-body problem to an effective one-body problem, to the (admittedly not very gender-neutral) problem of finding the “optimally happy” configuration of an ensemble of males and females with complicated interpersonal interactions (see Fig. 1): this is clearly much more easily tackled if one can replace it by an effective problem where only one female has to be moved while five males remain stationary. Another silly analogy that makes an effective point is comparing the use of pseudopotentials in electronic structure calculations to the effects of placing a cardboard cutout of a traffic policeman by the highway, in an effort to fool motorists into slowing down: it pretty much works, if done well enough, but is much cheaper!
6. Asking Questions

It goes without saying that, for students to learn effectively, it is important that they be encouraged to ask questions, and get into the habit where they examine critically whatever they have been taught. For both of these purposes, I have found it useful to make use of on-line sites such as “socrative” [9]. Despite the already mentioned digital divide, mobile phones are now extremely widespread throughout the developing world, and many developing countries now have a density of mobile phones (per population) that is similar to that seen in developed countries. With the advent of smart phones, both the instructor and the student can log on to such a website, which can then be used for rapid polling of the class as the lecture or hands-on session progresses, using either multiple choice questions or true/false questions, with immediate feedback in the terms of bar charts (similar to the operation of “clickers” which are used in some schools and colleges in the West).

For the teacher, the advantage of making use of such a tool is that one can get continuous feedback about whether or not concepts have been conveyed across adequately, and grasped accurately. One can then use this feedback to tailor the rest of the lecture accordingly. The responses from students to making use of such polling tools have been uniformly positive. Students say that they like the fact that it is interactive, and also the fact that it offers the opportunity to answer anonymously, since many students say they are otherwise reluctant to speak up in class, being put off by the fear of public “shame” or ridicule.

7. Hands-on Sessions and a “Massively Parallel” Calculation

The hands-on sessions require a room where students can work on computers either singly or in pairs, while guided through exercises by a tutor. Since students tend to have widely different paces of progress, it is important to have self-contained and clear instructions online, that students can follow at their own speed, if they wish to work faster, or are unable to keep up with the tutor.

The generally followed practice is to have a room full of students working through routine exercises in order to compute standard properties such as the lattice constant of silicon, or the vibrational frequency of carbon monoxide. This can seem like a huge waste of intellectual and computational power! For this reason, one can instead experiment with having students work on similarly simple but novel calculations – the typical such “massively parallel” research problem
would be one that would require performing a large number of quick calculations, each of which can be done by either one student or a small group of students.

At a summer school held in Bangalore in 2006, we followed this approach, asking students to address the problem of whether carbonia (the extended form of CO$_2$) can be stabilized by doping with silicon. Within a few days, the students were exposed to all the different steps one has to go through in order to tackle such a problem, from reading the literature, to formulating the problem and planning out calculations, performing various convergence tests with respect to basis set size and Brillouin zone sampling, etc. One question that arises is what would happen if students (who, after all, are beginners) should make a mistake? We decided to handle this by assigning every calculation to two to four pairs of students – if all the results agreed, it would be assumed that the result was correct, whereas if there was any discrepancy, then the calculation would be repeated and checked by a tutor or lecturer. We found that the students were incredibly enthusiastic about this project, and everyone involved was extremely delighted when this work resulted in a research publication [10], co-authored by 67 students, lecturers and tutors from all over the world!

8. Follow Up
In today’s digital society, it obviously makes sense to make full use of social media in order to keep students and lecturers connected during and after workshops. The participants of several workshops have stayed in touch through sites such as Facebook, and collaborations have been established through the contacts made. Many of the lectures from these workshops are also available online, and hundreds of students worldwide are making use of these resources.

9. Conclusions
In conclusion, I wish to reiterate that computational physics is an ideal field where students and researchers from developing countries can quickly and easily acquire the expertise to perform work that is of very high quality. However, there are traps and pitfalls for the uninitiated, and thus there is a great need for workshops and online resources that can help interested scientists to use the widely available computer packages appropriately and effectively. In this article, I have given some thoughts about how to do this, based on my experience in teaching in such workshops over the past two decades.

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