

qchem.qc-edu.org

- Lecture notes
- Assignments (& Solutions)
- Practice Problems (for extra credit)
- Syllabus
- Learning Objectives
- Reference Materials

Google Colaboratory

- Jupyter assignments
- Jupyter course notes

The screenshot displays the website qchem.qc-edu.org. The page is titled "Quantum Chemistry" and features a cat logo. The main content area is divided into several sections: "OVERVIEW" with a "Detailed Learning Objectives" link, "TOPICS" listing 10 items from GitHub to Many-electron systems, "ASSIGNMENTS" with 3 items, "EXTRA CREDIT" with an "Overview" link, "ADDITIONAL RESOURCES" with a "Reference Materials" link, and "CONTRIBUTING AND USING" with "Code of Conduct" and "How to Contribute" links. The right sidebar contains a "Contents" menu with links to "Overview", "Assessment", "Other resources", and "Using and Contributing". The "Overview" section includes a "CHEM 3PA3 Quantum Mechanics and Spectroscopy" description, a "Course Introduction video and slides" link, a "Syllabus" link, a "Marking Scheme" link, and "Learning Objectives" which are listed as: "Know, understand, and use the key equations of quantum mechanics for chemical applications", "Understand and apply the key concepts of quantum chemistry", "Read, write, and use common quantum chemical notation", "Know the ground-state wavefunctions, eigenenergies, quantum numbers, and selection rules for important exactly-solvable Hamiltonians. Be able to use these systems to (approximately) model real atomic and molecular systems", and "Know, understand, and apply quantum concepts to atoms & molecules". The "Assessment" section states that assignments will be turned in using GitHub Classroom and that extra points may be earned by making pull requests. The "Other resources" section includes a curated selection of material and a link to the 2021 course material at qchem1.qcdevs.org.

It's a beautiful day in Hamilton Ontario, and I hope you are well.

The purpose of this video is to provide an orientation to CHEM 3PA3.

First, CHEM 3PA3 is designed to introduce you to quantum mechanics, emphasizing the bits that are important for chemists.

The course content is online, both delivered and consumed asynchronously. There are online notes, assignments, and reference materials. It's all on the course web site, qchem.qc-edu.org.

The Million-Dollar Question



This course has a strange structure, which I should justify. When I was preparing, I kept asking myself: "What value can I add—what value can McMaster add—to the stuff you can find online." Because if you are motivated to learn quantum chemistry, there is an enormous amount of material online and in libraries; there are beautiful online video lectures; there are YouTube videos of people meticulously solving intricate problems. So what is my role? What is McMaster's role? I mean, why the hell are you paying tuition if everything is online for free? Why not do the online MIT course? I know the instructor for that course and, goshdarnit, Troy Van Voorhis is amazing!

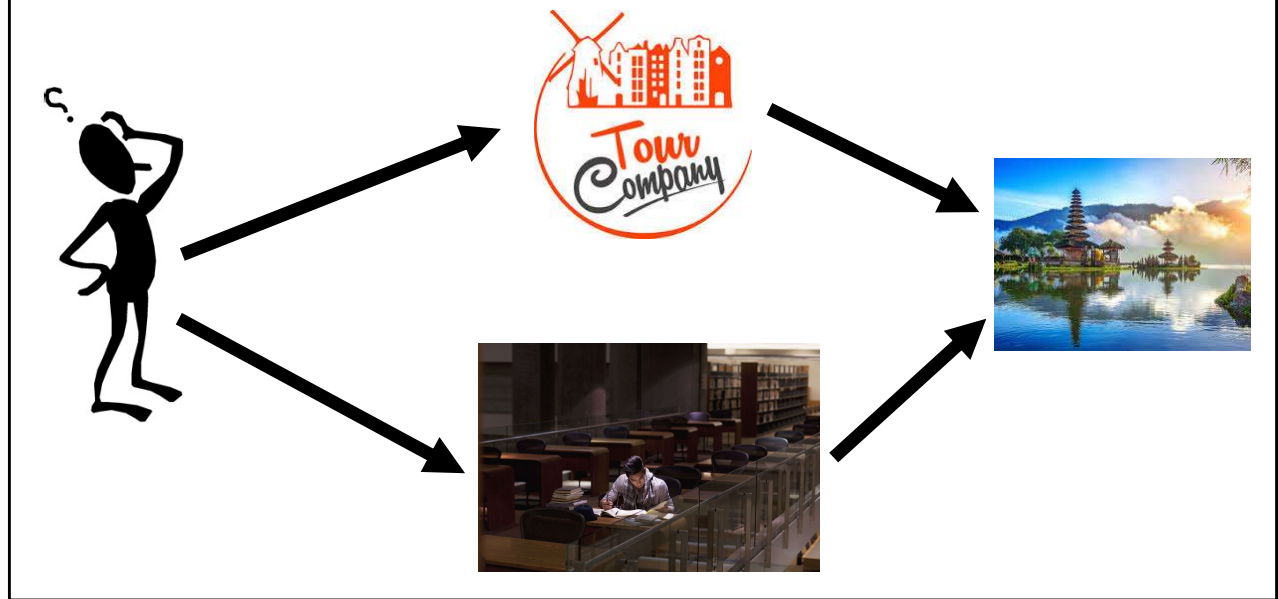
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The Million-Dollar Question

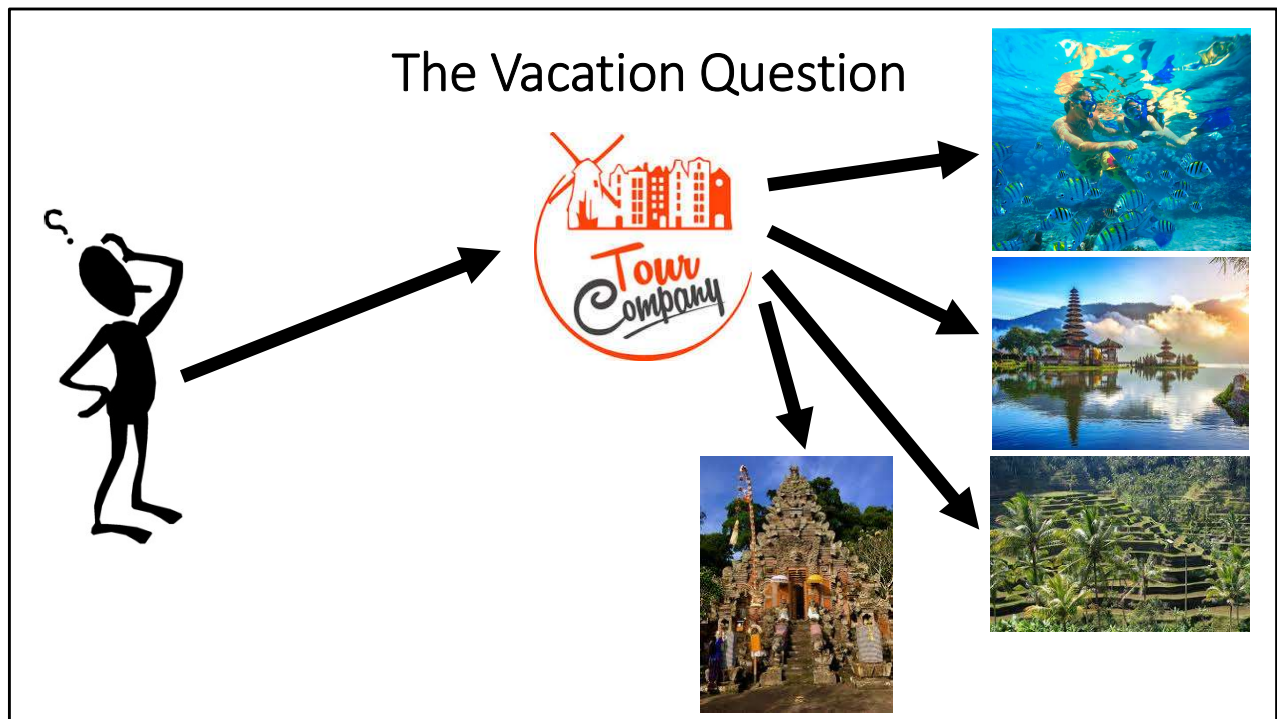


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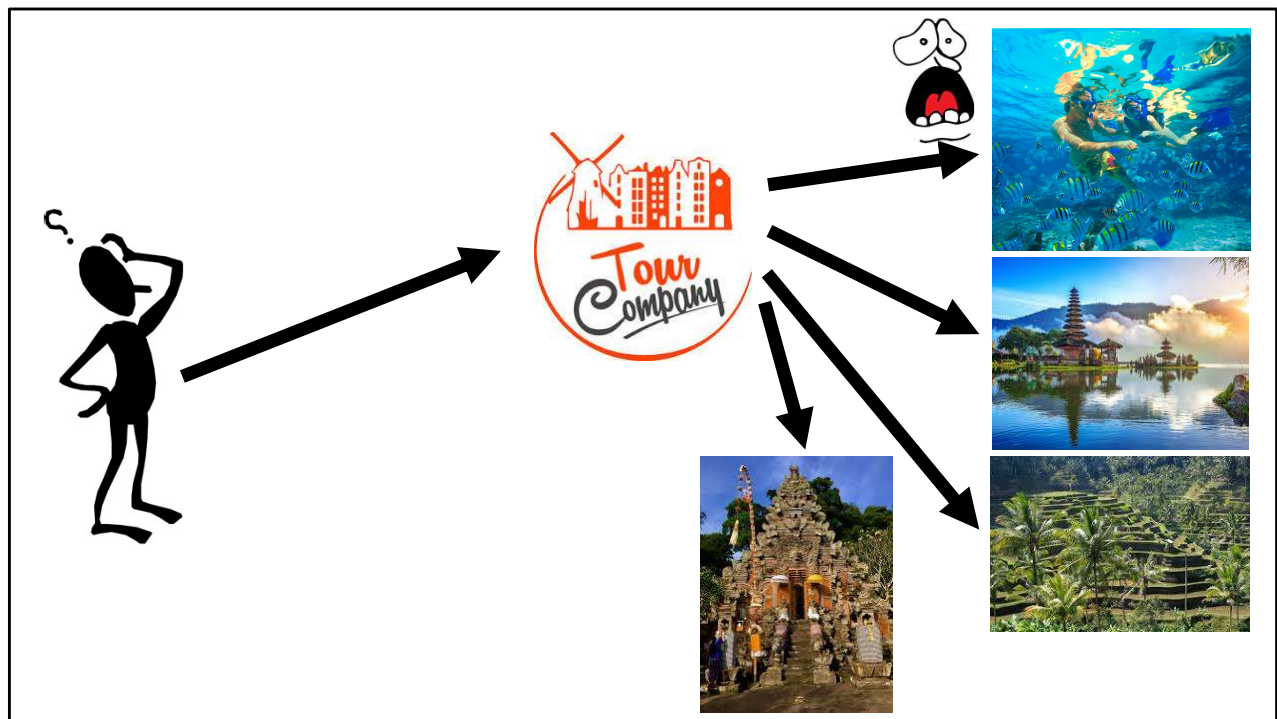
The Vacation Question



So how do I, and by extension McMaster, add value to the content you can find online? This is a hard question, so let's start with an easier one: when folks go on a trip, why do they hire a tour company? Why do they use a tourguide? I mean, if you are motivated to take a trip to, say, Bali, aren't you eager to read all about it on the internet, and watch all the videos about the amazing things you can see and do there? And if you were say, merely required to take a trip to Bali for a business conference (don't laugh, it happens), wouldn't you still want to do research so you could optimize your experience?

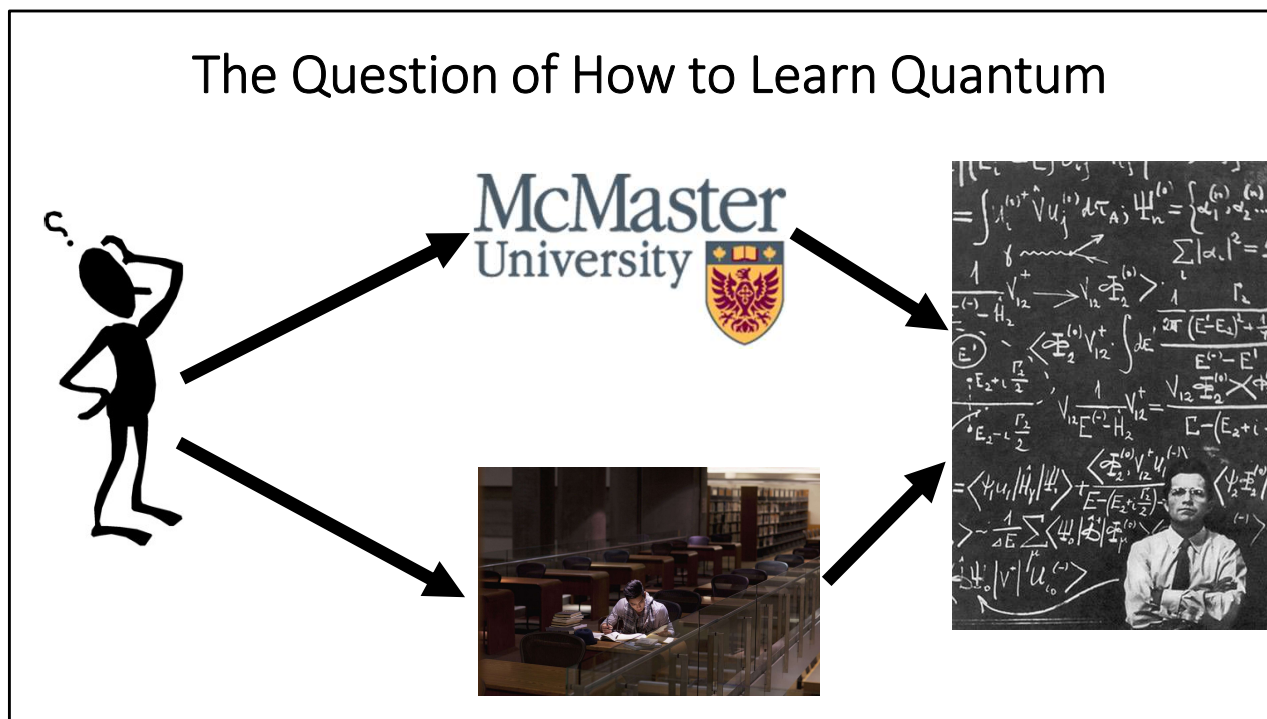


Well, I think that part of the problem is that the sheer quantity of information out there is intimidating. You want a tour company to hire someone who can somehow help you focus your search: after all, you don't want to do a Ph.D. on Bali, you just want to enjoy a nice long vacation there. So, by analogy, the university has hired a team of professors (your academic tourguides) to show you around chemistry, which is the vacation destination you chose to spend four of the best years of your life exploring.



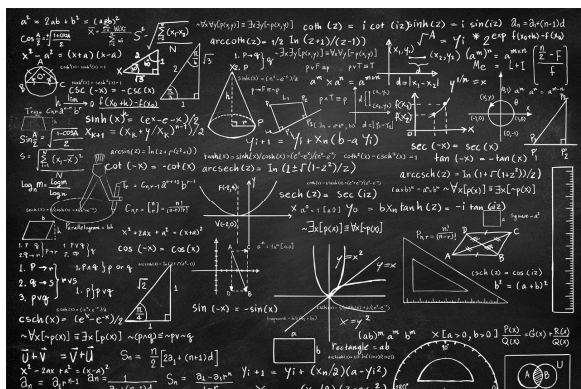
Now, alas, because you didn't do all the research yourself, you have to suffer through the fact that the tour company believes that there are certain things you should do, because otherwise you won't have truly experienced Bali. So you may have thalassophobia, but the tour company believes that you can't fully experience the beauty of Bali without going snorkeling. Similarly, the university believes that you can't be fully educated in chemistry without being exposed to quantum mechanics. I'm sorry if you have quantumphobia but ... think of this course as exposure therapy.

The Question of How to Learn Quantum



So what is my job then? Well, I'm your tourguide. If I were taking you snorkeling, it would be my job to teach you a few key techniques, lead you to a few interesting spots to explore, and point out a few ecologically important and/or aesthetically amazing phenomena. I can't swim for you, but I can make sure you are well-equipped to swim, and that your eyes are prepared for what you will see. By key quantum concepts and phenomena for chemical applications, and (3) help you notice especially important points. I can't learn for you, but I can make sure you are well-equipped to analogy, I see my job here as (1) teach you a few key techniques for quantum mechanics, (2) expose you to learn, and that your mind is prepared for what you'll be exposed to.



I still haven't answered the question I'm avoiding. If the university is like the academic tour company, and I am like the tourguide, you can still ask: why not just learn this myself. Well ... uh ... y'know, I think that's fine. You can do the research on quantum chemistry for yourself, and I've tried to make it easy for you by linking to **a lot** of valuable resources on the course web site and providing tons of practice problems. So it's cool. In fact, it's preferable: you'll work harder and learn more! Maybe you'll miss a few things I like, just like a person who goes to Bali and picks out their own snorkel spots might fail to see a manta ray. But you'll do fine. At the end of the course, after the exam, I'll interview you and if it's obvious you learned a lot of different, but equally important, content, then I'll give you a high grade and write you an excellent letter of reference.




But let's suppose you want to participate in my tour of quantum chemistry. What's my tour like? Well, I've observed that the biggest obstacle for most people in the course is the mathematics. And, y'know, most of you won't need to be excellent in mathematics in your future career. Let's go back to the analogy: it would be optimal if everyone who went to Bali were an expert swimmer certified in scuba diving.



But, hey, you can see most of the best stuff wearing a snorkel mask, flippers, and vest on the surface. So instead of teaching you the mathematics, we're going to use Jupyter. Now Jupyter is still something to learn, but it's something more broadly useful to chemists. I think that after you learn Jupyter, you'll never use Excel again...or at least not very often. You might not even use Microsoft Word that often, except for really fancily formatted documents. So the key technique to the course is Jupyter notebooks.



Quantum Chemistry

Search this book...

Quantum Chemistry

OVERVIEW

Detailed Learning Objectives

TOPICS

1. GitHub
2. Basics of Jupyter, Python, and Programming
3. From Newton to Schrödinger
4. The Schrödinger Equation
5. The Particle in a Box
6. Particles confined in two and three dimensions
7. The Postulates of Quantum Mechanics
8. 1-electron atoms
9. Approximate Methods

Quantum Chemistry

CHEM 393S Quantum Mechanics and Spectroscopy: An introduction to quantum chemistry and its applications in spectroscopy and structure and unusual phenomena at the nanoscale. The main course content is conveyed through, and assessed by, Jupyter notebooks, and uses the JupyterBook toolbox. GitHub Classroom is used for assessments.

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- Using and Contributing

Overview

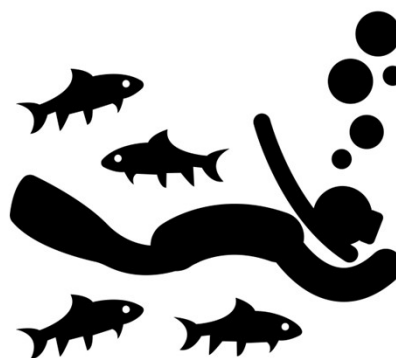
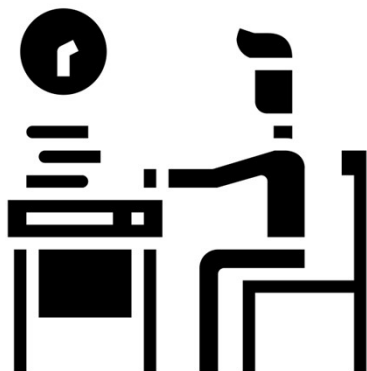
- **Course Introduction** video and slides.
- **Syllabus**
- **Marking Scheme**
- **Learning Objectives:**
 - Know, understand, and use the key equations of quantum mechanics for chemical applications
 - Understand and apply the key concepts of quantum chemistry
 - Read, write, and use common quantum chemical notation.
 - Know the ground-state wavefunctions, eigenenergies, quantum numbers, and selection rules for important exactly solvable Hamiltonians. Be able to use these systems to (approximately) model real atomic and molecular systems.
 - Know, understand, and apply quantum concepts to atoms & molecules.
 - Know, understand, and apply approximate computational strategies and their associated practical computational methods

Assessment

qchem.qc-edu.org



After we have a bit of exposure to Jupyter, the next step is to jump into the material. Each topic will have a Jupyter notebook, which is a jumping-off-point—a location I've chosen where there are interesting things to see. I'm not going to duplicate all the stuff that's online, or in books, or even in my own course notes. Most topics will also have a little video-introduction. Think of this as an orientation about what you'll see when you look beneath the surface of the topic.

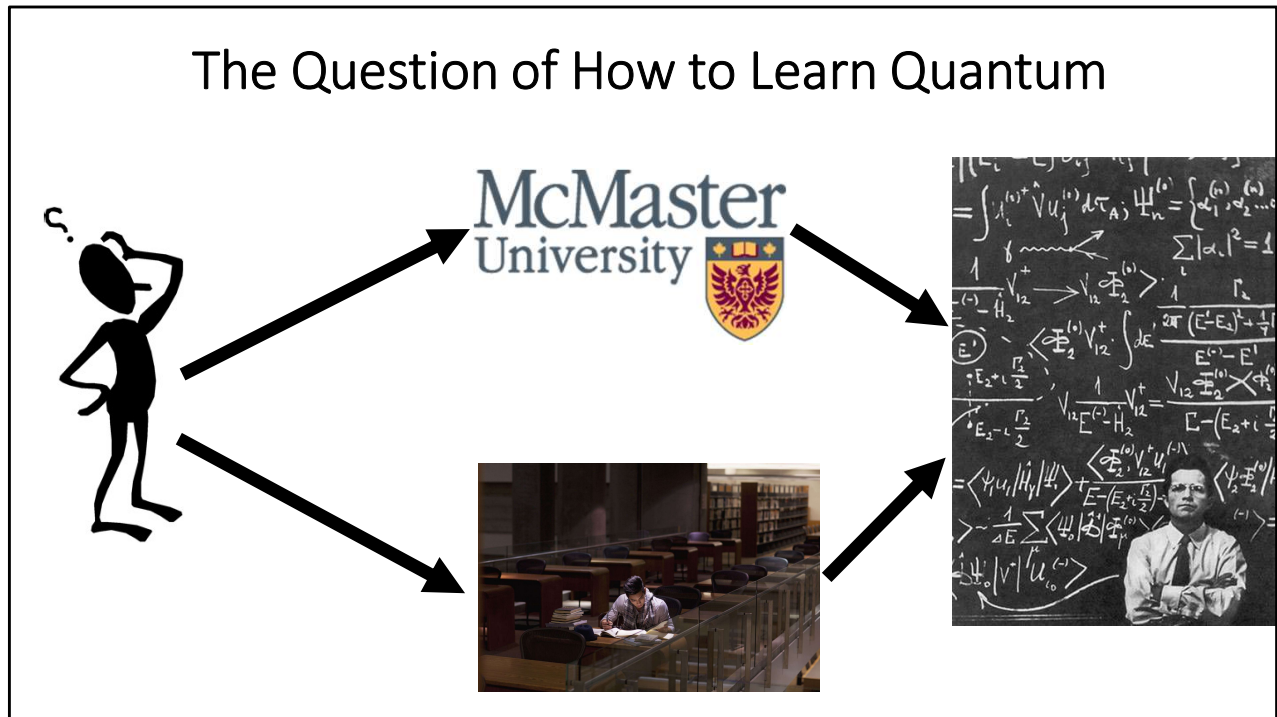


Now, just as you don't become an expert at Balinese snorkeling by sitting in the boat looking at pictures of coral and fish, you don't become an expert on quantum chemistry without doing it. So I've provided a lot of problems on the web site, and I'll provide some graded assignments too. You don't have to do my assignments. Just like you can learn an enormous amount about aquatic life in Bali without doing any tourguide-suggested activities, you can learn an enormous amount about quantum chemistry by immersing yourself in the material and thrashing away at problems until problems become easy for you. The more effort you expend engaging with the material, the more you'll learn, and I want to reward you for that. So you can submit the problems you do for extra credit.

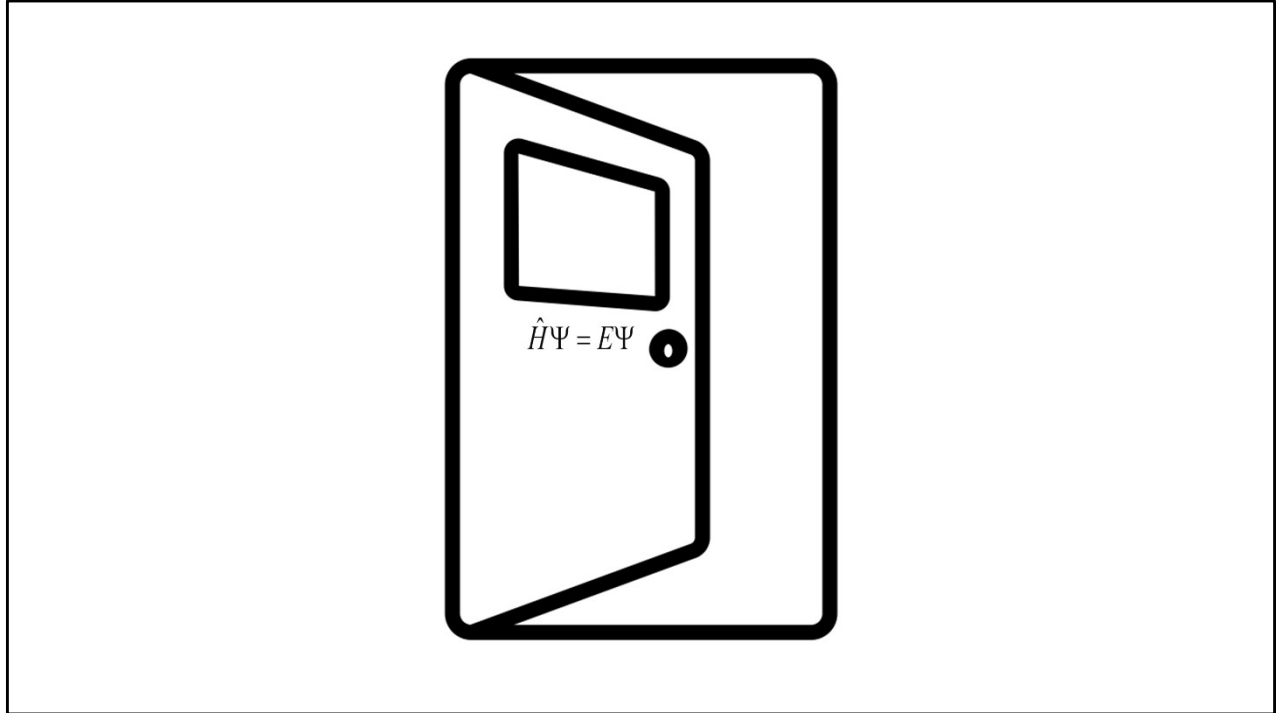


But I'm ****still**** dodging the question. Why are you paying for this course? What does McMaster do that is special or useful? What do I provide that is special or useful? Because I'm repeatedly admitting that not only is there nothing very special about me or McMaster, and I'm making it clear that if you learn the material in some other way I'm going to respect and reward that with the same credential McMaster would normally provide. This question is a lot deeper than this course; it has to do with the entire future of higher education. If the goal of your studies is to "get a piece of paper that leads me to a good job" then... Well, professional success is usually attributed to (a) skill, (b) luck, (c) work. Your innate skill is what you were born with, so please thank your mom and dad for that. Luck is, well, intrinsically uncontrollable. So you only control how you work, and while your diploma, or a high grade in this course, may help you find an opportunity, what you do with that opportunity will hinge on how hard—and how smart—you work. Alas, I don't control your skill, your luck, or your work. Neither I, nor anyone at McMaster, can learn for you, nor can we help you achieve professional success. So how can I be useful? Well, I can (try to) help you work efficiently so that you can learn more.

The Question of How to Learn Quantum



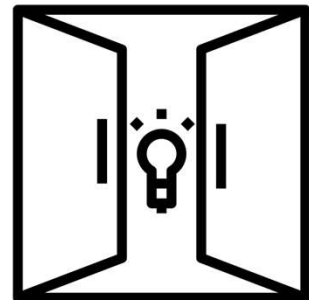
So how can I help you work smarter? Well, I have curated materials that I think are useful, to save you time exploring for yourself. But lots of people do that, and you can find similar collections all over the internet. Why should you use my materials instead of someone else's. To be honest, ****you shouldn't****. When I was taking difficult courses, I would always go to the library, find the appropriate section, and then I'd sit on the floor and go through all the texts on a given topic, selecting those that I found most understandable. My way of presenting this course material may not be right for you. You may find another way that's better for you and if you do, I want you to use it. I am **happy** if you curate your own approach to the course material. I **prefer** for you to learn the material in the way that works best for you, **especially** if that way is very different from what the way I'm leading the course.



But...I'm still dodging the question. What value **do** I contribute as an instructor? This is a hard question, so let's start with an easier one. If you go on a vacation and after a few days you realize that you don't really like your tourguide, why do you stick around? Hmmmm...a while back I went on a trip with my parents for their 50th wedding anniversary. We had a tourguide who, honestly, we weren't very impressed with. We would often go to one of the other tourguide's orientation lectures, but in the end, when we were actually on location, we were with our assigned tourguide. And that was OK. She was available; she was helpful; she was knowledgeable. Maybe she wasn't the best fit for my family's background and interests, but she was **there** with us, and no one else was. We could have wandered off on our own but having someone to whom we could ask questions, having someone who could point out where our preconceptions were wrong...that was valuable. So we stuck around.

So I believe the **only** thing that I can contribute to this course is **myself**. Because you can find great materials online and in the library, but you can't write those people a message and expect a reply; you can't go to those people's office and ask them questions. I may not be the best at this stuff, but I'm **here**, and they're not. Therefore, my main method of instruction in this course is one-on-one interactions. Ask me, or the TA, questions about the material; ask us questions about other people's materials; ask me questions about snorkeling in Bali. I'm here as a resource for you. McMaster put us here. We may not be the best fit for your background or interests, but we're available; we're helpful; we're knowledgeable.

~20 Billion* The Million-Dollar Question



*** Estimated size of the global higher education industry.**

P.S. In the end, I still haven't really answered the big hairy question: why should you pay tuition? The past, present, and future of the university is merely this: you pay to have access to a community of scholars who are committed to helping students learn. I believe that McMaster's troupe of tourguides is among the best in the world, even if some universities have more **prima ballerinas** and **danseurs noble**. That's because the most knowledgeable scholars are not necessarily the best educators and even if they were...well, most people can't afford to hire Fabien Cousteau as a snorkel guide for their Balinese vacation.