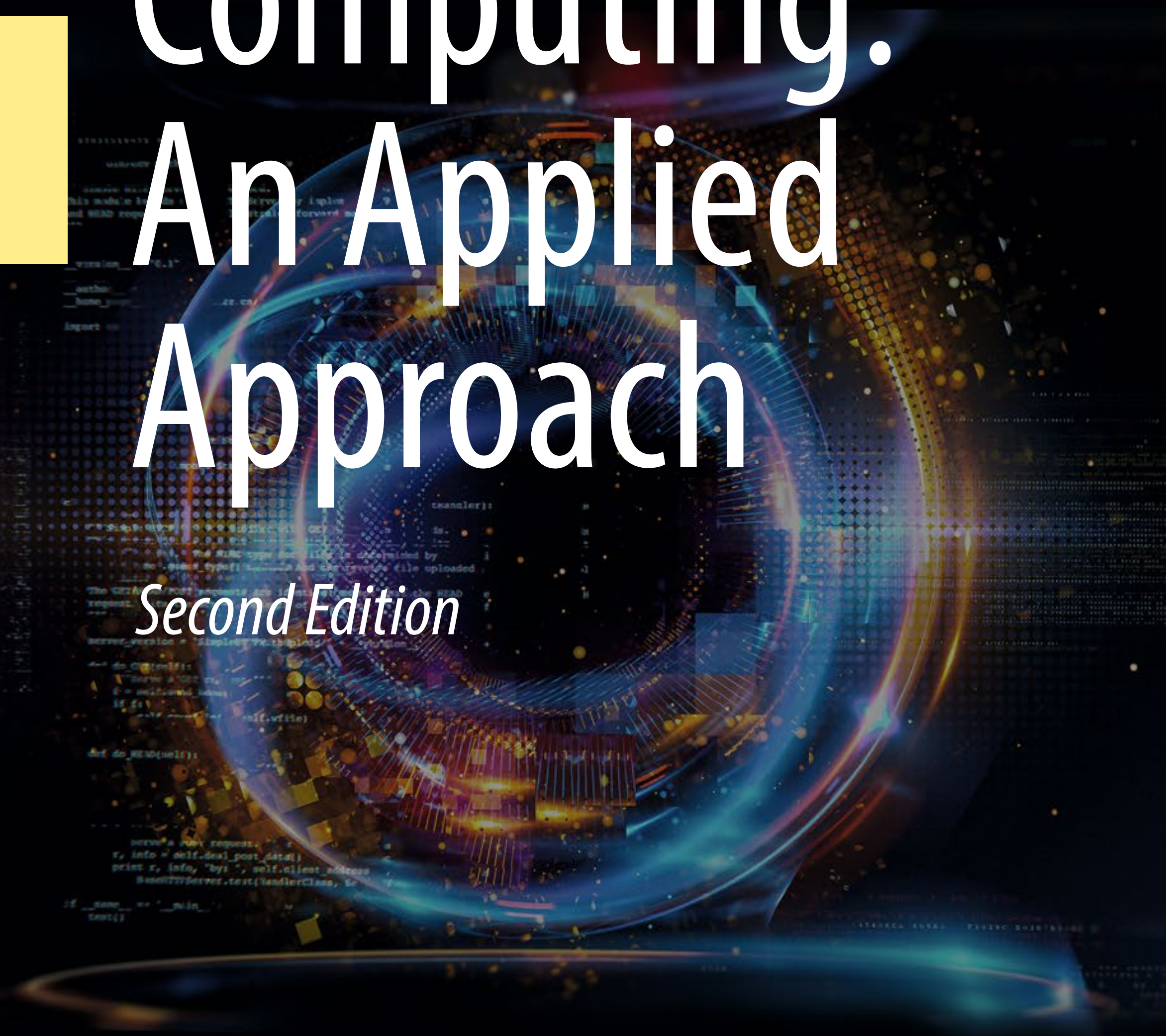
Jack D. Hidary

Quantum Computing: An Applied Approach

Second Edition



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Preface to the Second Edition

The field of quantum computing has grown rapidly in the two years since the first publication of this book. The first page of the book went through five printings in its first year which mirrors the growing number of individuals ramping up in the sector. I would like to thank all the faculty, students and other readers from so many countries who provided helpful input for this new edition.

Our world, of course, changed in many other ways as well since the publication of the first edition. The global pandemic impacted all areas of society and will probably transform how we work together for years to come. While in-person meetings were halted, quantum tech researchers and engineers found ways to continue their collaborations online.

In the last year, many countries have announced new or expanded quantum tech initiatives. These programs are injecting significant resources into the quantum tech ecosystem. We have also noted the rise in private investment in the sector – both in quantum computing hardware companies as well as various applications startups. All this activity has sharply increased the demand for individuals who are trained in quantum computing as well as those with additional hands-on experience in coding for these machines. This, in turn, has led many universities to launch and expand their quantum information science curricular programs and for corporations to start quantum tech training programs for their teams.

With this new edition I continue to strive towards the goal of making quantum computing more accessible to a wider range of individuals. This is a technical book, but one that I hope opens the door to quantum computing for individuals who would like to get a rigorous grasp of how to make these novel computing devices work and which kinds of problems we should focus on when using these platforms.

This second edition contains several updates and expanded areas of coverage, including:

- Expanded coverage of quantum machine learning and quantum error correction
- Expanded chapter on principles of quantum mechanics
- Updated chapter on quantum hardware
- Coverage of the QSVT framework
- New chapter on Dirac notation
- This new edition also corrects known typos from the first edition (thankfully, there were not many). If any new typos have entered into the second edition please make a note of them in the online site.
- All the code throughout has been re-tested and updated for the current versions of the various quantum computing frameworks and libraries.

All of these additions and updates are based on requests from readers. The companion online site for the book is also updated and I recommend that readers check the site for a range of resources including updated downloadable code, problem sets and further instructional material.[1]

I look forward to all the creativity that will emerge in this field and the positive impact the discipline will have on so many important fields. Please continue to send in your input via the online site.

Jack D. Hidary
September 2021

[1] http://www.github.com/jackhidary/quantumcomputingbook

Preface to the First Edition

We are entering a new era of computation that will catalyze discoveries in science and technology. Novel computing platforms will probe the fundamental laws of our universe and aid in solving hard problems that affect all of us. Machine learning programs powered by specialized chips are already yielding breakthrough after breakthrough.

In this book we will explore quantum computing – an emerging platform that is fundamentally different than the way we compute with current digital platforms. To be sure, we are years away from scaled quantum computers. Yet, we now know that such systems are possible; with advances in engineering we are likely to see real impact.

Quantum computing is part of the larger field of quantum information sciences (QIS). All three branches of QIS – computation, communication and sensing – are advancing at rapid rates and a discovery in one area can spur progress in another. Quantum communication leverages the unusual properties of quantum systems to transmit information in a manner that no eavesdropper can read. This field is becoming increasingly critical as quantum computing drives us to a post-quantum cryptography regime. We will cover quantum teleportation and superdense coding, which are both quantum-specific protocols, in chapter 7.

Quantum sensing is a robust field of research which uses quantum devices to move beyond classical limits in sensing magnetic and other fields. For example, there is an emerging class of sensors for detecting position, navigation and timing (PNT) at the atomic scale. These micro-PNT devices can provide highly accurate positioning data when GPS is jammed or unavailable.

In this book we will focus on quantum computation. One of the critical differences between quantum and classical computation is that in quantum computation *we are manipulating quantum states themselves*; this gives us a much larger computing space to work in than in classical computers. In classical computers, if we wish to model a real-world quantum physical system, we can only do so with representations of such a system and we cannot implement the physics itself.

This key difference leads to exciting possibilities for the future of computing and science. All this starts with fundamental truths about our world that were developed during the quantum mechanics revolution in the first half of the 20th century. We will review a number of these core concepts in the first chapter.

I had the fortunate circumstance to have studied quantum mechanics before learning classical physics and therefore relate to quantum physics as the norm – it is my intellectual home. Until we change our educational system, most students will learn the classical before the quantum and so the quantum will seem doubly strange — both from their own human experience as well as from the inculcation of classical ideas before quantum ideas can be introduced.

What is ironic about this state of affairs is that the primary mathematical tool in quantum mechanics is linear algebra, a powerful but very accessible branch of mathematics. Most students, however, only take linear algebra after two or three semesters of calculus, if they take it at all. Yet, no calculus is needed to introduce linear algebra! In any case, we will leave the remedying of mathematics education to another day while we embark here on a journey into a new form of computing.

In this book we will explore how to build a computer of a very different kind than humans have ever built before. What is distinct about this book is that we will go beyond the theoretical into the practical work of how we can build such computers and *how we can write applications for these systems*. There are now several development libraries which we can use to program cloud-based quantum systems. We will walk through code examples and show the reader how to build a quantum circuit comprised of a set of operators to address a particular challenge. We will mainly use Python in this book.

We are currently in the regime of **n**oisy **i**ntermediate-**s**cale **q**uantum (NISQ) computers, a term coined by John Preskill of CalTech [224]. This refers to systems that do not yet have full error-correction (thus noisy) and have dozens to thousands of qubits – well short of the 10^6+ necessary for scaled fault-tolerant computing. Despite the limitations of these initial systems, the theory, algorithms and coding techniques we cover in this book will serve readers as they transition to larger systems that are to come in the future.

This work is three books in one: the first part covers the necessary framework that drives the design of quantum computers and circuits. We will also explore what kinds of problems may be amenable to quantum computation in our treatment of complexity classes.

The second part of the book is for those readers who wish to delve into the programming that makes these new machines tick. If you already have a background in quantum mechanics, quantum information theory and theoretical computer science (you know who you are!), you can jump right to the second part and dig into the code. Please refer to the navigation guide in the following pages to chart a course through this material.

In the third part we provide a set of critical tools to use in the journey to master quantum computing (QC). We build up the core concepts of linear algebra and tie them specifically to their use in QC. The table of operators and circuit elements in chapter 15 is a handy reference as you design your own quantum computing protocols.

The book is also a portal to the growing body of literature on the subject. We recommend that the reader use the bibliography to explore both foundational and recent papers in the field.

We will provide further online examples and code tutorials on a continual basis. This is a living text that will develop as QC technology matures. We are all travelers together on this new adventure; join us online at this book's GitHub site.[2] We are excited to see what you will develop with these new platforms and tools. Contact us via the site — we look forward to hearing from you.

Jack D. Hidary
June 2019
35,000 ft up

[2] http://www.github.com/jackhidary/quantumcomputingbook

Acknowledgements

Let me start by thanking my publisher, Elizabeth Loew, who has been so supportive throughout the process, and the entire SpringerNature team for their excellence.

A book like this is a significant undertaking and it took a team of people to help in so many ways. The greatest of appreciation to Stefan Leichenauer who did a great job as book editor and formatter-in-chief. Stefan reviewed large parts of the book and I thank him for his commitment to the project. The entire book is written in TeX and we often pushed the boundaries of what TeX is capable of implementing.

Thank you to Sheldon Axler, author of *Linear Algebra Done Right* (also by Springer) who generously shared his TeX template so that we could format the book correctly for the Springer standards.

Thanks to the many experts who gave of their time to review key sections of the book and provide technical advice. These include (in alphabetical order): Scott Aaronson, Ryan Babbush, Sergio Boixo, Ruffin Evans, Eddie Farhi, Patrick Hayden, Gerry Gilbert, Matt Reagor and Lenny Susskind. Each improved the work materially with their input.

I would also like to recognize the significant achievement of Michael Nielsen and Isaac Chuang in developing their textbook [206]. Recognition as well to John Preskill for his in-depth lecture notes [222]. Nielsen, Chuang and Preskill as well as Mermin [194] and Rieffel [236] have helped many individuals enter the field.

Thanks to my many colleagues at Alphabet, Google, Sandbox and X who have encouraged this effort including: Sergey Brin, Astro Teller and Hartmut Neven and his excellent team.

Thank you to the many participants in the workshops I taught on quantum computing as well as my courses on linear algebra and other mathematical topics. Your feedback has been invaluable.

Hearty thanks to James Myer who worked with me intensively on the math sections; James' methodical approach assured us of success. We reviewed these sections countless times, continually reworking them. James is not only passionate about mathematics; he also cares deeply about pedagogy and we had productive discussions on the best way to present the core concepts. Thank you as well to Tai-Danae Bradley who also reviewed the math sections and made very helpful suggestions.

Thank you to Ryan LaRose who worked with me on the code sections. In this emerging field where the code frameworks have only been developed within the last few years, solid information and examples can be hard to come by. Ryan combined great skill in research as well as compiling the information in succinct forms. Ryan also did a great job on the book's GitHub site.

Thank you to Ellen Cassidy who did such a professional job proofreading the text for grammar and consistency of format. Ellen has an eagle eye and I commend her work to any author. Joe Tricot also did a wonderful job coordinating the overall process. Thanks also to Nathan Schor and Sam Ritchie for their eagle eyes on typo corrections for the second edition.

Naturally, even with all this help, there will remain items to fix for the next edition. All remaining errors are mine and I will be posting updates on the GitHub site and then include fixes in upcoming versions.

Thank you to my parents, David and Aimee Hidary, and my entire wonderful family for their support through this process. It is a great feeling to share this accomplishment with you.

Navigating this Book

Here are our suggestions to make the best use of this book:

1. *University instructors:* You can build several different courses with the material in this book. All code from the book is on the book's website. The math chapters have exercises embedded throughout; for other chapters please consult the online site for coding exercises and other problem sets.
   (a) Course in Quantum Computing for STEM majors:
      i. For this course we recommend assigning chapters 1 and 2 as pre-reading for the course and then proceeding chapter by chapter with the exercises provided on the GitHub site. Solutions are also available on the site.
      ii. If the students do not have sufficient depth in formal linear algebra and related mathematical tools, Part III forms a strong basis for a multi-week treatment with exercises.
   (b) Course in Quantum Computing for physics graduate students:
      i. For this course, we recommend using this book in conjunction with Mike and Ike (which is the way many of us refer to Nielsen and Chuang's excellent textbook [206]) or another suitable text which covers the theoretical concepts in depth. We all owe a huge debt of gratitude to Michael Nielsen, Isaac Chuang and authors of other textbooks over the last twenty years. We also recommend referring to John Preskill's lecture notes as you build your course for advanced physics students [222]. Our work is meant to be complementary to Mike and Ike in several respects:
         A. This work is more focused on coding. For obvious reasons, books written prior to the past few years could not have covered the dev tools and Python-based approaches to quantum computing that now exist.

B. This book does not go into the depth that Mike and Ike does on information theoretic concepts.
C. This book's mathematical tools section has a more detailed ramp-up for those students who may not have taken a rigorous linear algebra course. The short summaries of linear algebra and other requisite math tools in other textbooks on quantum mechanics are often insufficient in our experience.

ii. We recommend first assigning chapters 1 and 2 as pre-reading.
iii. Next, we suggest covering the chapters on unitary operators, measurement and quantum circuits with exercises on the Github site to check knowledge.
iv. We then recommend spending the bulk of the course in Part II to provide the students with hands-on experience with the code.

(c) Course in Quantum Computing for CS graduate students:

i. We suggest assigning the first two chapters as pre-reading and then a review of mathematical tools in Part III. Prior exposure to only undergraduate linear algebra is typically insufficient as it was most likely taught without the full formalism.
ii. We then recommend chapters 3 and 4 to build up familiarity with unitary operators, measurement and complexity classes in the quantum regime. The instructor can make use of the review questions and answers on the GitHub site.
iii. The course can then cover the approaches to building a quantum computer followed by all the coding chapters.

Please check the book's GitHub site to find additional resources including: code from the book, problem sets, solutions, links to videos and other pedagogical resources.

2. *Physicists:* For physicists who specialize in fields outside of quantum computing and wish to ramp up quickly in this area, we recommend reading the brief history of QC as we provide more detail than typical treatments, then the survey of quantum hardware followed by the applications in the second part of the book.
3. *Software engineers:* We recommend starting with the opening two chapters, then reviewing the toolkits in Part III. We then suggest returning to the treatment of qubits and unitary operators in Part I and proceeding from there.

4. *Engineering and business leaders:* For readers who will not be doing hands-on coding, we recommend focusing on chapters 1- 4. The more adventurous may want to work through some of the code examples to get a tangible feel for the algorithms.
5. *Independent study:* This book can easily be used as a text for independent study. We recommend combining it with online resources. Please consult the GitHub site for an updated list of resources:

   http://www.github.com/jackhidary/quantumcomputingbook

   We recommend first assessing your current fluency on the core tools in Part III; there are numerous self-tests throughout the section that can be used for this purpose. The reader can then proceed to Part I.

   For those with a strong background in quantum mechanics and/or information theory we recommend looking up the papers referenced in chapters 2- 4 to gain a deeper understanding of the state of the field before proceeding to Part II: Hardware and Applications.

Please consult the book's GitHub site to find a range of resources including: code from the book, problem sets, solutions, links to videos and other pedagogical resources.

Part I

Foundations

CHAPTER 1

Superposition, Entanglement and Reversibility

What is a quantum computer? The answer to this question encompasses quantum mechanics (QM), quantum information theory (QIT) and computer science (CS).

For our purposes, we will focus on the core of what makes a quantum computer distinct from classical computers.

1.1 Quantum Computer Definition

A quantum computer is a device that leverages specific properties described by quantum mechanics to perform computation.

Every classical (that is, non-quantum) computer can be described by quantum mechanics since quantum mechanics is the basis of the physical universe. However, a classical computer does not take advantage of the specific properties and states that quantum mechanics affords us in doing its calculations.

To delve into the specific properties we use in quantum computers, let us first discuss a few key concepts of quantum mechanics:

- How do we represent the superposition of states in a quantum system?
- What is entanglement?
- What is the connection between reversibility, computation and physical systems?

We will be using Dirac notation, linear algebra and other tools extensively in this text; readers are encouraged to refer to the math chapters later in this work as well as chapter 14 on Dirac notation to review as needed.

J. D. Hidary, *Quantum Computing: An Applied Approach*,
https://doi.org/10.1007/978-3-030-83274-2_1

1.1 *Superposition and Entanglement*

According to the principles of quantum mechanics, systems are set to a definite state only once they are measured. Before a measurement, systems are in an indeterminate state; after we measure them, they are in a definite state. If we have a system, for example, that can take on one of two discrete states when measured, we can represent the two states in Dirac notation as $|0\rangle$ and $|1\rangle$. We can then represent a *superposition of states* as a linear combination of these states, such as

$$\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \tag{1.2}$$

1.3 The Superposition Principle

The linear combination of two or more state vectors is another state vector in the same Hilbert space[a] and describes another state of the system.

[a] See Part III for a treatment of Hilbert spaces

As an example, let us consider a property of light that illustrates a superposition of states. Light has an intrinsic property called *polarization* which we can use to illustrate a superposition of states. In almost all of the light we see in everyday life — from the sun, for example — there is no preferred direction for the polarization. Polarization states can be selected by means of a *polarizing filter*, a thin film with an axis that only allows light with polarization parallel to that axis to pass through.

With a single polarizing filter, we can select one polarization of light, for example *vertical polarization*, which we can denote as $|\uparrow\rangle$. *Horizontal polarization*, which we can denote as $|\rightarrow\rangle$, is an orthogonal state to vertical polarization[1]. Together, these states form a basis for any polarization of light. That is, any polarization state $|\psi\rangle$ can be written as linear combination of these states. We use the Greek letter ψ to denote the state of the system

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\rightarrow\rangle \tag{1.4}$$

The coefficients α and β are complex numbers known as *amplitudes*. In this example, the coefficient α is associated with vertical polarization and the

[1] We could have equally used $|0\rangle$ and $|1\rangle$ to denote the two polarization states; the labels used in kets are arbitrary.

coefficient β is associated with horizontal polarization. The amplitude has important interpretation in quantum mechanics which we will see shortly.

After selecting vertical polarization with a polarizing filter, we can then introduce a second polarizing filter after the first. Imagine we oriented the axis of the second filter perpendicular to the axis of the first. Would we see any light get through the second filter?

If you answered no to this question, you would be correct. The horizontal state $|\rightarrow\rangle$ is orthogonal to the first, so there is no amount of horizontal polarization after the first vertical filter.

Suppose now we oriented the axis of the second polarizing filter at 45° (i.e., along the diagonal $\nearrow$ between vertical $\uparrow$ and horizontal $\rightarrow$) to the first instead of horizontally. Now we ask the same question — would we see any light get through the second filter?

If you answered no to this question, you may be surprised to find the answer is *yes*. We would, in fact, see some amount of light get through the second filter. How could this be if all light after the first filter has vertical polarization? The reason is that we can express vertical polarization as a *superposition* of diagonal components. That is, letting $|\nearrow\rangle$ denote 45° polarization and $|\nwarrow\rangle$ denote $-45°$ polarization, we may write

$$|\uparrow\rangle = \frac{1}{\sqrt{2}}|\nearrow\rangle + \frac{1}{\sqrt{2}}|\nwarrow\rangle \tag{1.5}$$

As you may expect from geometric intuition, the vertical state consists of equal parts $|\nearrow\rangle$ and $|\nwarrow\rangle$.

It is for this reason that we see some amount of light get past the second filter. Namely, the vertical polarization can be written as a *superposition* of states, one of which is precisely the 45° diagonal state $|\nearrow\rangle$ we are allowing through the second filter. Since the $|\nearrow\rangle$ state is only one term in the superposition, not all of the light gets through the filter, but some does. The amount that gets transmitted is precisely $1/2$ in this case. (More formally, the intensity of the transmitted light is $1/2$ that of the incident light.) This value is determined from the amplitudes of the superposition state by a law known as Born's rule, which we now discuss.

1.2 *The Born Rule*

Max Born demonstrated in his 1926 paper that **the modulus squared of the amplitude of a state is the probability of that state resulting after**

measurement [47]. In this case, since the amplitude is $\frac{1}{\sqrt{2}}$, the probability of obtaining that state is $\left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$, so the probability of measuring the light in either the vertical or horizontal polarization state is 50%. Note that we chose an amplitude of $\frac{1}{\sqrt{2}}$ in order to *normalize* the states so that the sum of the modulus squared of the amplitudes will equal one; this enables us to connect the amplitudes to probabilities of measurement with the Born rule.

1.6 The Born rule

In a superposition of states, the modulus squared of the amplitude of a state is the probability of that state resulting after measurement. Furthermore, the sum of the squares of the amplitudes of all possible states in the superposition is equal to 1. So, for the state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, we have

$$|\alpha|^2 + |\beta|^2 = 1.$$

While in the polarization example above we have a 50/50 split in probability for each of two states, if we examined some other physical system it may have a 75/25 split or some other probability distribution. One critical difference between classical and quantum mechanics is that amplitudes (*not probabilities*) can be complex numbers.

In other words, the coefficients α and β which appear in the statement of the Born rule can be complex numbers, such as $i := \sqrt{-1}$ or $(1 + i)/\sqrt{2}$. It is only after we take the square of the modulus of these amplitudes that we get real numbers, hence actual probabilities. Refer to chapter 11 to review complex numbers and how to calculate the square of the modulus of a complex number. As if quantum superposition were not interesting enough, QM describes a specific kind of superposition which stretches our imagination even further: *entanglement*. In 1935, when **E**instein worked with **P**odolsky and **R**osen to publish their paper on quantum entanglement, their aim was to attack the edifice of QM (this paper is now known as EPR [100]). Even though Einstein earned the Nobel Prize for his 1905 work on the quantum nature of the photoelectric effect, he nevertheless railed against the implications of QM through his later years.

Einstein wrote in 1952 that quantum mechanics appears to him to be "a system of delusion of an exceedingly intelligent paranoiac concocted of incoherent elements of thought" [99]. He hoped that the EPR paper would demonstrate what he perceived to be the deficiencies of QM.

EPR showed that if you take two particles that are entangled with each other and then measure one of them, this automatically triggers a correlated state of the second — even if the two are at a great distance from each other; this was the seemingly illogical result that EPR hoped to use to show that QM itself must have a flaw. Ironically, we now consider entanglement to be a cornerstone of QM. Entanglement occurs when we have a superposition of states that is not separable. We will put this into a more formal context later on in this text.

This "spooky action at a distance" seems at odds with our intuition and with previous physics. Podolsky, the youngest of the co-authors, reportedly leaked the paper to the New York Times to highlight this assault on the tower of QM to the public. The Times ran the story on the front page of the May 4th, 1935 edition with the headline “Einstein Attacks Quantum Theory."

Not only is entanglement accepted as part of standard quantum mechanics, we shall see later in this work that we can leverage entanglement to perform novel types of computation and communication. From an information theoretic point of view, entanglement is a different way of encoding information. If we have two particles that are entangled, the information about them is not encoded locally in each particle, but rather in the correlation of the two.

John Preskill likes to give the analogy of two kinds of books: non-entangled and entangled [224]. In the regular, non-entangled book we can read the information on each page as we normally do. In the entangled book, however, each page contains what appears to be gibberish. The information is encoded in the correlation of the pages, not in each page alone. This captures what Schrödinger expressed when he coined the term entanglement:

> Another way of expressing the peculiar situation is: the best possible knowledge of a whole does not necessarily include the best possible knowledge of all its parts. [249]

Schrödinger further noted that in his opinion entanglement was not just *one* of the phenomena described by quantum mechanics,“but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought” [249].

1.7 Entanglement

Two systems are in a special case of quantum mechanical superposition called *entanglement* if the measurement of one system is correlated with the state of the other system in a way that is stronger than correlations in the classical world. In other words, the states of the two systems are not *separable*. We will explore the precise mathematical definitions of separability and entanglement later in this book.

1.3 *Schrödinger's Equation*

As we saw above, we can represent the state of a system with a state vector using Dirac notation. For example, if we wish to represent the state of a system of one photon that is in a superpositon of vertical and horizontal polarization we can use the following notation

$$|\nearrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\rightarrow\rangle \tag{1.8}$$

We can also represent the state vector with the Greek letter Ψ in the ket – recall that the label in the ket is arbitrary. So we now have

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\rightarrow\rangle \tag{1.9}$$

If we measure this photon for polarization we have a 50% probability of finding the photon in a vertical polarization state and 50% probability of finding it in a horizontal polarization state. In the Copenhagen school of QM we say that the wave function has collapsed to one state or the other. There are other interpretations of measurement of quantum systems, but these are beyond the scope of this text.

Now that we have a method of representing the state of a system with a wave function, how can we represent the evolution of this system through time? For this exposition, let us consider the wave function of a particle that is moving through free space which we can represent as

$$\Psi(x, t) \tag{1.10}$$

where x is its position at time t. The manner in which this wave function evolves over time can be described by the time-dependent Schrödinger equation (SE). One conventional way of writing down the time-dependent SE for a particle along one dimension is as follows

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t) \tag{1.11}$$

There is no need to be intimidated by this mathematical notation if it is new to you. We will explain the core concepts of the SE here and the reader can find links to helpful videos on our companion website for deeper exploration of the SE.

On the left hand side (LHS) of this equation, we see the constants i and $\hbar$. i of course is the symbol that represents the square root of -1. $\hbar$ is the reduced form of the Planck constant h. We call it the reduced form since we take h and divide it by 2π. The next set of symbols is the partial derivative of the wave function ψ with respect to t which denotes time. A partial derivative with respect to time refers to how the function, in this case the wave function $\Psi(x,t)$, will change as t changes while holding position, denoted as x, constant.

The right hand side (RHS) of the equation denotes the Hamiltonian operator applied to the wave function Ψ. The Hamiltonian represents the total energy of a system; the total energy includes all the kinetic energy, which we can represent as $\hat{T}$ and the potential energy, $\hat{V}$, of the particles in the system. Note that some conventions use $\hat{U}$ instead of $\hat{V}$ to denote potential energy, but we avoid that here to reserve U for the generic reference to unitary operators which we will encounter later in this book.

An operator is a term we introduce in quantum mechanics for functions that operate on wave functions. In addition to the Hamiltonian operator we often encounter the position and momentum operators in QM which are represented as $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$, respectively. Note the carat on top of these operators to distinguish them from the position and momentum variables, x and p.

The SE tells us that if we want to know how the wave function Ψ will change over time we need to look at the total energy of the system. We can break down $\hat{H}$ to its component parts of $\hat{T}$ and $\hat{V}$ like so

$$\hat{H}\Psi = \hat{T}\Psi + \hat{V}\Psi \tag{1.12}$$

We can then replace $\hat{T}\Psi$ with the quantized version of the expression for kinetic energy. We start with the classical formula for kinetic energy

$$T = \frac{1}{2}mv^2 \tag{1.13}$$

then we can multiply both the numerator and denominator by m on the RHS and then realize that since momentum, p, is mass times velocity, we yield the following

$$T = \frac{(mv^2)m}{2m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m} \tag{1.14}$$

Now we can take this classical expression and upgrade it to its quantum counterpart by replacing p with the momentum operator $\hat{\mathbf{p}}$ which is

$$\hat{\mathbf{p}} = -i\hbar\frac{\partial}{\partial x} \tag{1.15}$$

Since in equation 1.14 we have p^2 we replace it like so

$$\hat{T} = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right) \tag{1.16}$$

To simplify the RHS, we can do the following: realize that the $-i$'s cancel out to -1 so cancel those out and add a minus sign to the front of the RHS, then collect the two $\hbar$'s to a single $\hbar^2$ and finally multiply out the two first order partial derivatives to yield a second-order partial derivative as follows

$$\hat{T} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right) \tag{1.17}$$

Now let's turn to the LHS. Since we use the Schrödinger equation to calculate the evolution over time of the wave function, we represent this by the partial derivative of the wave function, $\Psi(x, t)$, with respect to t like so

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} \tag{1.18}$$

We now can put all the pieces together as follows

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + \hat{V}\Psi(x,t) \tag{1.19}$$

Voila! Now, what about the term $\hat{V}\Psi(x, t)$? This term has to be determined for the system at hand. Let us consider the case of a quantum harmonic oscillator. The potential energy of a harmonic oscillator such as a spring is described by the following expression

$$V = \frac{1}{2}kx^2 \tag{1.20}$$

where k is the spring constant of the oscillator. We then recall that