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VIEWPOINT

Quantum computing and probability

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Abstract
Over the past two decades, quantum computing has become a popular and promising approach to trying to solve computationally difficult problems. Missing in many descriptions of quantum computing is just how probability enters into the process. Here, we discuss some simple examples of how uncertainty and probability enter, and how this and the ideas of quantum computing challenge our interpretations of quantum mechanics. It is found that this uncertainty can lead to intrinsic decoherence, and this raises challenges for error correction.

1. Introduction

A new computing paradigm has appeared over the past couple of decades—quantum computing. This concept brings together ideas from information transmission, computer science, quantum physics, and quantum electronics (including optics) [1]. Quantum computing has become of interest due to the suggestion that it provides a methodology by which very rapid computations may be achieved with no dissipation [2]. In general, the speed of these computations has been compared to that of classical, sequential digital computers in which a single processor is used. Indeed, the speed of quantum computing has promised the prospect of factoring large integers into their prime factors [3], a task that is known to be computationally hard on classical computers. The primary difference between the bits on a classical digital computer and the qubits of a quantum computer is that the latter incorporate quantum mechanical phase factors that allow a continuous range of projection onto the '0' and '1' states. As such, the qubits themselves should be thought of as analog objects. That is, the state is a continuous (complex) variable, basically the phase of the complex qubit, instead of merely a '0' or a '1'. Yet, a quantum computer, like a classical computer, is a set of interconnected processing elements, but now the latter are a set of qubits. The efficacy of the quantum computation scheme lies in the ability to build in efficiencies through the use of quantum entanglement [4].

The attraction of quantum computation has been strong, and it originally grew out of the feeling that this was an approach to reversible computation, where no energy would be dissipated in the computing process [5]. Here, it was presumed that qubit transitions from one gate to the next would follow by the use of unitary transformations, as (textbook) quantum mechanics was closed and dissipation free. In general, one can easily do logical reversibility, but there is a difference between logical reversibility and physical reversibility[1] [6]. Even in the case of logical reversibility, one must be concerned about whether this is compatible with probabilistic flow through the gates. That is, the flow of information through the qubit gates in a quantum computer represents the evolution of a quantum system. Quantum mechanics is a probabilistic theory [8], and one has to worry about how this intrinsic probability affects quantum computation.

To illustrate these points, consider the simple quantum circuit in figure 1. This circuit depicts a portion of a quantum computing circuit, in which a controlled ϕ-rotation gate and a Hadamard transform gate are indicated to act upon three qubits, denoted by the vectors on the left. In addition, the instantaneous state of the system is indicated by the wavefunctions along the bottom. In general, as in all such discussions of quantum circuits, the process, or information, flow is assumed to move from the left to the right. In these circuits, then, the quantum evolution in some sense has a trajectory[2] that moves from the left to the right, and for which the coherence of the wavefunction is assumed to be maintained throughout the computation. Then, it must be assumed that a preferred arrow of time has been imposed upon the system, and

[1] Originally, Landauer [7] showed that erasing information meant physical irreversibility, but the converse is not true. Avoiding the erasure of information does not imply physical reversibility. In fact, the prototypical (logically reversible) quantum gate, the Toffoli gate, can easily be implemented with traditional (dissipative) CMOS gates. In essence, logical reversibility is necessary, but not sufficient for a reversible computer.

[2] While Dirac [9] discussed trajectories for quantum mechanics, his concept involved projection onto a sequence of eigenvalues. This will reappear later in the discussion.

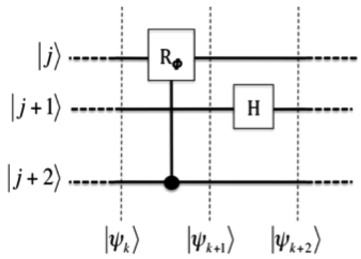

Figure 1. Part of a quantum computing circuit. The instantaneous state of the system is indicated by the wavefunction at the bottom and the particular qubit is denoted by the left-hand kets.

this reflects upon the reversibility of the system, as such time asymmetry is usually coupled to dissipation.

Of more interest for our current purpose, one must ask how these circuits are affected by uncertainty and probabilistic behavior. For example, if we assume that the indicators along the bottom of the circuit in figure 1 correspond to a spatial progress of the information, then the unitary operation leads to a change of phase of the qubits as one moves through the circuit. But, this is a spatial change of the phase, the latter of which incorporates the velocity or momentum of the qubit's wavefunction. This quantity does not commute with the spatial position assumed in the circuit, and the resulting uncertainty clearly affects the results of the indicated operations[3]. Born [8] provided the probabilistic view for quantum mechanics, in which the expectation value of an operator is an average over a great many 'trials' of the evolution of this wavefunction, in essence expressing the need for an ensemble averaging process. Yet, the quantum circuit is thought of as being the single processing entity. But, the statistical errors in this approach may well be such that the gate operation will lead to conditions which are not plausible and the circuit cannot be implemented [10]. It is this point that we want to examine, and shall do this with some very simple examples which effectively illustrate the nature of the problem.

Having posed the problem, some caveats must be faced. Estimating intrinsic errors from uncertainty relations, which is the approach suggested, is known to give very small numbers [11]. Nevertheless, this gives a break with fully reversible behavior and is still important. We will return to the ensemble idea later.

In the following sections, we first discuss some simple qubit operations corresponding to the quantum circuit of figure 1, and assess the role of probability there. We then turn to the point that quantum computing challenges our common interpretation of quantum mechanics, so that we have to examine other interpretations to obtain a clear picture of what is really happening. Finally, we discuss how this may affect schemes which are designed to overcome error through qubit encoding.

2. Qubits and probability

The question is about how probability affects the qubits that arise in quantum computing, such as those in figure 1. In this figure, we have two gates. The question is how probability will enter the framework of this quantum circuit. Do we assign a probability p that the qubit is in state $|1\rangle$ and a probability $q = 1 - p$ that the state is in state $|0\rangle$, or do we assign a probability p that the quantum evolution to the right occurs and a probability q that it does not occur? These are very simple questions, but get right to the heart of the role of probability in quantum computing.

2.1. The controlled phase gate

In the first scenario, we consider the controlled phase gate in figure 1. Here, the state of the two qubits are taken to have the space

$$|j+2, j\rangle \rightarrow \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}, \tag{1}$$

and the qubit transition matrix reads

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\varphi} \end{bmatrix}. \tag{2}$$

That is, when the $j + 2$ qubit is in the 1 state, a phase is applied to the 1 state of the j qubit. This is a unitary matrix representing the unitary transformation applied to the wavefunction. In general, if we have a combination of states in the $j + 2$ qubit, we get, for example,

$$\begin{aligned} (\alpha|0\rangle + \beta|1\rangle)_{j+2}|0\rangle_j &\rightarrow \alpha|00\rangle + \beta|10\rangle, \\ (\alpha|0\rangle + \beta|1\rangle)_{j+2}|1\rangle_j &\rightarrow \alpha|01\rangle + \beta e^{i\varphi}|11\rangle. \end{aligned} \tag{3}$$

Here, $|\alpha|^2 + |\beta|^2 = 1$. These two quantities tell us the fraction of each initial state that is present, presumably from a previous gate, but they cannot be put into the transition matrix (2). Otherwise, this would break the unitarity of this matrix. The presence of an error in the input state, say the probability of a different combination, will change the α and β. For example, if these two were reversed in position, the phase of the qubit would change its sign. Without loss of generality, we may rewrite the input combination as

$$\alpha = \frac{1}{\sqrt{2}}, \qquad \beta = \frac{1}{\sqrt{2}}e^{i\vartheta}. \tag{4}$$

A very simple model for an error might then be to use

$$\begin{aligned} \alpha' &= p\alpha + q\beta = \frac{p + qe^{i\vartheta}}{\sqrt{2}}, \\ \beta' &= p\beta + q\alpha = \frac{q + pe^{i\vartheta}}{\sqrt{2}}. \end{aligned} \tag{5}$$

Here, $p + q = 1$. If α' and β' remain normalized, then we would only have an error propagation. But, we cannot guarantee this is the situation. In fact, the inner product results in

$$p^2 + q^2 + 2pq\cos(\vartheta), \tag{6}$$

which only retains normalization for one value of the angle ($\vartheta = 2n\pi$). Had we chosen $p^2 + q^2 = 1$, the normalization

[3] The use of position and momentum here is arbitrary, as most qubit operations will entail non-commuting operators at some point. Thus, those chosen here can be taken as generalized operator pairs.

problem would not have gone away, although the angles at which it remains would be shifted. Even if the combination remains normalized, so the signal will propagate properly to the output of the gate, the error will also propagate through the gate. Thus, the error does not remain localized to this particular gate.

In a classical gate, small errors are reset to 0 or 1 by the nonlinearity in the gate function itself. The level that constitutes 'small' is defined by the noise margin in this nonlinear switching function. But, the quantum gates are linear, so that there is no natural reset process, and the errors will propagate through the gate and the remaining gates of the system.

Here, we have not addressed the problem of whether or not the unitary transition matrix (2) is completely applied in the process, as mentioned above. We leave this to the following discussion.

2.2. The Hadamard gate

Similarly, in the second scenario above, we will use the Hadamard gate as an illustration. In figure 1, the Hadamard transformation is applied to qubit $j+1$. This transformation has the form

$$\mathbf{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{7}$$

This is a unitary transformation. The issue here is the time at which the transformation is 'complete'. As we mentioned, the phase incorporates the conjugate variable, such as the momentum. Hence, the uncertainty relation suggests that an uncertain momentum means an uncertain time at which the transform is complete. The possibility of this range of times is discussed more below. Here, for the probabilistic situation, we will again use a very simple model. We assume that the unitary transformation occurs with probability p, so that the Hadamard matrix is multiplied by p and an $\mathbf{I}_2$ matrix, which represents no operation occurring, is multiplied by q. When these are added, the net matrix is also no longer unitary. This will be detailed further in the discussion below, where we find both an amplitude and a phase error. For the present, we are led to the conclusion, that probability does not seem compatible with the unitary transitions envisioned for the individual qubits. How do we reconcile this with the idea of the quantum computing circuit?

3. Are quantum circuits reasonable?

We mentioned that a preferred arrow of time had been introduced in figure 1, in the assumption that the information (or processing) flow was from the left of the figure to the right of the figure. The presence of this arrow of time in computation is considered to imply that the system is in a non-equilibrium state [12]. Generally, this implies dissipation and decoherence in the system, a recognition reflected in DiVincenzo's call for long decoherence times in quantum computing [13]. But, the 'information flow' in figure 1 raises new questions with quantum mechanics itself, as this is an introduction of causality or determinism, which is incompatible with the normal interpretation of quantum mechanics[4]. Yet, here we have a quantum computational process that seems to require just what is not supposed to be present. Thus, we must either give up our quantum circuit or find an alternative interpretation of quantum mechanics.

A further question is how does the consideration of probability within the gate square with the common (Copenhagen) interpretation of quantum mechanics, in which *measurements* tend to introduce probabilities. That is, the statistical behavior lies only in the classical world. Now, is this a problem with quantum computing, or a problem with the common interpretation of quantum mechanics? Since the very advent of quantum mechanics, there have been arguments over whether or not it was a complete theory [16]. These arguments have continued to this day. Indeed, Ghose [17] summarizes a number of situations in which the common interpretation seems inadequate. Here, we seem to require an interpretation of quantum mechanics which admits to a causal, deterministic flow. One such interpretation is that of de Broglie [18] and Bohm [19] (dBB). Another is the consistent histories approach of Griffiths [20]. We discuss this latter first.

3.1. Consistent histories

In common quantum mechanics, wavefunction collapse is considered the byproduct of measurements. In contrast, wavefunction collapse in the consistent histories approach is a mathematical procedure for calculating conditional probabilities within the quantum evolution [21]. Probabilities are introduced as part of the axiomatic foundations of quantum theory, irrespective of measurements. We can think of a history as a sequence of alternatives at a specific set of times [22]. These alternatives may be simple yes/no statements, but open the door for probabilities at each state. Thus, the states $|\psi_k\rangle$ in figure 1 may each be characterized by a 'probability' P_k for the possible states. In the strictest interpretation, this probability is a projection operator which takes the entire Hilbert space to the allowed set of states [23], and so a trajectory in the spirit of Dirac [9] is introduced. By nature, these projection operators compress the phase space and introduce decoherence, which is why the consistent histories approach is often called the decoherence approach. But, now questions about time and determinism become almost irrelevant.

In moving from one state to the next in figure 1, it may be assumed that there is a time ordering in the states, with $\cdots t_k < t_{k+1} < t_{k+2}\cdots$, etc. In turn, the system evolves via the Hamiltonian, and a particular history can be written as [24]

$$H = (\cdots P_{j+2}P_{j+1}P_j\cdots), \tag{8}$$

where P_i is the probability that proposition i is true at t_i. In the Hilbert space, we then have to introduce projections onto the desired space, and propagators from one state to the next,

[4] Bohr asserted that quantum mechanics '... implies a renunciation as regards the causal space-time coordination ...' [14]. Born is more explicit in this regard, stating that '... in the quantum theory it is the principle of causality, or more accurately that of determinism, which must be dropped ...' [15].

which leads to

$$H = [\cdots \hat{P}_{k+1} U(t_{k+1}, t_k) \hat{P}_k \cdots], \tag{9}$$

where

$$U(t_2, t_1) = \mathrm{e}^{-\mathrm{i}H(t_2 - t_1)/\hbar} \tag{10}$$

for a time independent Hamiltonian.

Herein lies the problem discussed above. The last equation assumes that we can define a specific time to each of the states along the bottom of figure 1. But, as we pointed out previously, if we take these states as being spatially located in the quantum circuit (one possibility), then the operator (10) contains the momentum in the phase exponent and thereby suffers from the uncertainty relation. That is, the position and momentum do not commute, and the resulting uncertainty in momentum makes the time at which the 'trajectory', from state $|\psi_k\rangle$ to $|\psi_{k+1}\rangle$, actually arrive at this latter state uncertain. The result is that we cannot be sure that the operation has been completed at the designated time t_2 assigned to this latter state. This is the heart of the quantum error that is introduced in the Hamiltonian, as discussed in section 2.2 for the Hadamard gate. At the end of the process, the projection operator, or the probability it represents, picks out that fraction of states for which the Hadamard gate operation would have been effective. Hence, our probability that the operation was actually applied is transformed into the projection operation onto the set of states that would result from the Hadamard operation being successful.

We can demonstrate this for the Hadamard gate. For simplicity, we assume that the basis set at $|\psi_{k+1}\rangle$ is $\{|0\rangle, |1\rangle\}$, and then the desired Hilbert space after the Hadamard gate is

$$|\psi_{j+2}\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{bmatrix} \equiv \begin{bmatrix} u_0 \\ u_1 \end{bmatrix}. \tag{11}$$

In fact, with the uncertain transform $p\mathbf{H} + q\mathbf{I}_2$, the transformed state is given by

$$|\psi_{j+2}\rangle' = \begin{bmatrix} (q + \frac{p}{\sqrt{2}})u_0 + \frac{p}{\sqrt{2}}u_1 \\ (q - \frac{p}{\sqrt{2}})u_1 + \frac{p}{\sqrt{2}}u_0 \end{bmatrix}. \tag{12}$$

There are two important points to be made here. First, the amplitude is changed for each of the two states, and becomes

$$1 - (2 \mp \sqrt{2})p(1-p) \leqslant 1. \tag{13}$$

The non-unitarity results in reduction of the amplitude of the state, which of course introduces an error in the qubit. Secondly, however, the amplitude reduction differs for the two states, and this introduces a phase error in the qubit. This phase error is a different form of quantum error, which would not be encountered in classical bits. While much effort has been expended in discussing *extrinsic* decoherence arising from interactions with the environment, this is an *intrinsic* decoherence which has not been well discussed. We also note that the resulting probability that enters (12) for P_{j+2} is just p, as we might have suspected.

A final important point is that the errors are now moved to the possible values of the state, $|\psi_{k+2}\rangle$ in this case. Assigning a probability to the possible values of a qubit is just the assumption that we followed in the controlled phase gate of section 3.1. What we find is that the two possible sources of error described in section 3 seem to merge to the same resulting definition for error in the state, and this error occurs in both the amplitude and phase of the qubit. While the model may be quite simple, the important result is that the errors, both amplitude decay and dephasing, build upon one another and propagate through the gates.

3.2. The de Broglie–Bohm approach

The dBB theory arises through the introduction of pilot waves with trajectories, but is often thought of as a wave *and* particle theory. The key factor here is that it admits to a causal flow with probabilities (and uncertainty) confined to the initial conditions [25]. In general, the wavefunction is expanded into an amplitude and a phase S, and this then gives a deterministic equation for the general coordinate

$$m_i \frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{\partial S}{\partial x_i}. \tag{14}$$

This approach becomes a statistical theory with the assumptions that the *initial* values of the various x_i are distributed probabilistically according to some function on the configuration space of the system[5].

Here, one might even consider entanglement as a hidden variable. Entanglement is fundamental to quantum mechanics [29], and is the process by which quantum computing gains its power to process information with exponentially fewer resources than classical computing [30]. Yet, observation of the entangled state depends upon a very special tensor-product Hilbert space, whereas normally the expectation value of an operator is independent of the choice of basis set. This suggests that there is no operator which yields an expectation value that is a measure of entanglement [31, 32]. What remains then is to consider entanglement as a hidden variable. Quantum computing appears to be a natural scenario for invoking the dBB interpretation of quantum mechanics.

The problem with this view lies in the fact that the probability in dBB is restricted to the initial condition, and the resulting trajectories are deterministic. But, which trajectories? Leavens has pointed out that the initial distribution gives rise to a set of possible trajectories, and this in turn leads to an arrival time distribution [33]. This distribution corresponds to the uncertainty issue discussed above. Truncating at a finite time leads to error. In essence, this puts us in the same quandary as finding the value of (10) at the defined time of a particular state, as discussed above. If we are to use the dBB theory, then we have to think of discrete quantum propagations, in which each gate starts with an initial state with its own probability distribution. In this sense, the quantum circuit becomes quite meaningful, as each stage is a separate

[5] One objection to the dBB theory is that it is generally considered to be a 'hidden variable' theory, a situation which is thought to have been ruled out by the work of Bell [26]. However, Bell's theorem only applies to 'local' hidden variables, and has come into question itself recently [27], while the second is that Bell himself was a fan of the dBB theory [28].

propagation. At the same time, this begins to connect to the consistent histories approach[6].

There are other interpretations of quantum mechanics which also could be employed as well. There is the well-known 'many worlds' interpretation of Everitt [35]. Bell felt that this was basically a version of the dBB theory without trajectories [28], while Ghose viewed it as failing some tests, in that '. . . there is a conceptual proliferation of unrelated worlds at every observation' [17]. Thus, it seems that the two previous interpretations may well be the most useful for discussing the basis and application of quantum computing in a manner that allows the probability to occur.

4. Discussion

To summarize the above discussion, it is clear that the unitary transformations that describe the quantum gate contain a momentum operator, which from the uncertainty relation introduces a variation of the time at which the operation is complete. For example, the unitary transformation can be expressed by a Green's function that operates on the wavefunction, and this in turn can be expressed as a Feynman path integral [36]. The latter is a summation over all possible paths, or trajectories (such as those which occur in the dBB theory). These trajectories have a distribution of arrival times [33], so that any truncation at a finite time incurs an error in the Green's function/unitary transformation. This error has both an amplitude and phase component, and propagates from one state to the next, providing correlated error through the quantum circuit. Thus, there are intrinsic, internal errors within quantum gates.

To overcome general errors, it was suggested to use error correcting codes for quantum computing [37], and a great deal of effort has been addressed to this point. In fact, the basic premises upon which the use of error correction codes is based may have to be reconsidered. In general, it is assumed that such codes make it possible to correct for *some* of the qubits being corrupted in an unknown way [38]. First, it is assumed that the original qubits can be encoded by the application of a unitary transformation at the beginning [39]. But, the unitary transformation itself may introduce errors, as discussed above. How do we separate the quantum totality into an encoding part and a processing part? Even after the encoding, it is usually assumed that only a fraction of the qubits are affected by the decoherence, and that these errors are introduced independently of each other [37]. In fact, this means that the system may be fault tolerant if the errors do not propagate from one block to the next [40]. But, the results above suggest the opposite—the intrinsic errors propagate.

Kak [41] argues that the error correction concept is largely based upon concepts arising from classical computing, and that certain errors in qubits cannot be corrected. An example might be the case discussed above for the Hadamard gate. While a general loss of amplitude, due to decoherence, might be correctable, the fact that this loss is different for the two states of the qubit is problematic. It is not clear that the resulting phase error can be effectively corrected.

There is also the suggestion for the use of so-called decoherence free subspaces which decouple the qubit from its environment [42]. While we have shown there are errors that arise merely from the operation of the qubit transformation and are not environment-induced errors, it is not clear whether the decoherence free subspace will be as effective in this situation. Yet, at least one plan has been suggested for actually using weak interaction with the environment to stabilize qubits in the decoherence free subspace [43], an approach which clearly moves away from totally reversible computing.

We should return to the idea of ensembles, since one idea is to compute until we get it right, which has been suggested for single photon computing [44]. Also, the suggested cluster states, composed of large numbers of qubits, might also represent a meaningful ensemble approach [45]. These present different approaches, in which it is not immediately clear how the simple ideas presented here apply.

In summary, we have shown that probability within the computational steps is a source of intrinsic decoherence within the computational set of gates. Moreover, the lack of probability and the apparent causal, deterministic flow in quantum computing circuits drives us to consider alternative descriptions of quantum mechanics. It appears that this deterministic behavior in quantum circuits can be reconciled with quantum mechanics in a number of different interpretations, such as consistent histories and the dBB interpretation. As a result, it may be that quantum computing gives us new insight into the basics of quantum mechanics and constraints on any completeness in the theory.

[6] To be sure, there have been suggestions that these two approaches are inconsistent with one another, but Hartle has clarified the two approaches and where they differ [34]. The dBB theory allows for interference, but the consistent histories assumes that these interferences have disappeared due to decoherence. In this sense, consistent histories incorporates the Kolmogorov probability definitions, which do not admit the negative probabilities. If we ignore these interferences at the individual state level of the quantum circuits, such as figure 1, then there is little difference in the two approaches. It is important to note that this interference is not the same as entanglement. Rather, this interference arises from coherence between the initial state and the final state of each stage of the circuit, and can lead to e.g. phase errors due to circuit 'resonances'.

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