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NONLINEAR SCHRÖDINGER EQUATION FOR QUANTUM COMPUTATION

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Utilization of a quantum system whose time-development is described by the nonlinear Schrödinger equation in the transformation of qubits would make it possible to construct quantum algorithms which would be useful in a large class of problems. An example of such a system for implementing the logical NOR operation is demonstrated.

Keywords: Nonlinear quantum mechanics; quantum computation.

1. Introduction

Quantum computing algorithms[1] make use of the possibility of parallel operations on states which make up a superposed set. After appropriate operations have been made, a number of measurements may be carried out, resulting in the collapse of the wavefunction to a smaller set, from which information related to the solution of the particular problem may be deduced.

Emphasis in previous work on quantum computing algorithms has been on time independent unitary operations on the superposed states. Focus on such operations is natural, as the superposed states need to be associated with relatively simple quantum degrees of freedom, whose time development could be described by a Schrödinger equation incorporating a simple Hamiltonian. On the other hand, it was noted by Abrams and Lloyd[2] that a much richer set of problems can lend themselves to solution by quantum computation if nonlinear evolution of the qubit states could be realized. In particular, they demonstrate that the availability of a special nonlinear operation on a single qubit enables the construction of a quantum algorithm whose repetitive application results in efficient progressive separation of searched states from others. They also show that implementation of a two-bit nonlinear quantum AND gate allows for an algorithm which finds the answers to an NP-complete problem with certainty in linear time. It is indicated that the two-bit nonlinear transformation itself may be obtained through ordinary unitary operations in combination with single qubit nonlinear operations.

Such nonlinear single qubit operations have been studied in Refs. 3–7, with the emphasis being on the analysis of fidelity in obtaining the results of these operations through unitary transformations.

A possibility for realizing nonlinear quantum operations is through system dynamics described by the nonlinear Schrödinger equation which appears in the analysis of Bose–Einstein condensation[8] (BEC) and other contexts.[9]

Recent developments in the ability to experimentally control, manipulate, and detect these condensates[10,11] lend hope to the idea that it may indeed be possible to construct some building blocks for quantum computation utilizing this phenomena.

Shi[12] has demonstrated that nonlinear quantum evolution is possible in Bose–Einstein condensates coupled to one another through a tunneling junction. An explicitly nonlinear equation of motion for the containment well occupation coefficients has been derived. An important feature of this work is that it demonstrates how entanglement in BEC is realized, starting from fundamental considerations. The work also contains a discussion of the possibility of utilizing this nonlinearity in quantum computations.

Admittedly, these equations involve approximations, and appear only because the "background" in a collective quantum system is treated in some mean-field form. The discussion of the validity of the range of the approximation to a particular implementation may be deferred as a technical detail. However, the utilization of a (possibly macroscopic) collective quantum event as a qubit raises deeper questions which must be answered. We briefly touch upon this point in the concluding paragraph.

In this paper, we will assume that the dynamics of such nonlinear Schrödinger equations may be applicable to operations on qubits and look into the possibilities introduced by such operations. It will be shown that a two-qubit quantum gate can be constructed with a single condensate (in contrast to the more than one studied in Refs. 12–15) in the presence of a non-uniform potential. It will also be pointed out that the availability of such nonlinear quantum operations allow the efficient search for an optimal solution through pairwise elimination of possibilities making up an extended solution set.

2. Nonlinear Quantum Computation — An Application

A typical quantum computation algorithm utilizes the creation of a superposition of parallel states, usually a complete set of enumerable states:

$$|\Psi_1\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle \,. \tag{1}$$

If the qubits forming the pure state $|k\rangle$ is formed by n quantum states with two possible eigenstates each, then $N = 2^n$, and k may be taken as the number corresponding to the binary representation generated by the n qubits.

The space is then enlarged to include a function of k in the representation:

$$|\Psi_1\rangle \to |\Psi_2\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle|f(k)\rangle \,. \tag{2}$$

The extended space containing $|f(k)\rangle$ itself is made up of additional qubits. A measurement carried out on this state will yield a superposition of a smaller subset:

$$|\Psi_2\rangle \to |\Psi_3\rangle = \frac{1}{\sqrt{N'}} {\sum_k}' |k\rangle|f(k)\rangle \,, \tag{3}$$

where the prime on the summation indicates a sum over a subset of the states $|k\rangle$ consistent with the results of the measurement, a total number of N'. Similar operations involving enlargements of the space, unitary transformations on the superposed states, and measurements may be carried out until a final set of measurements will yield results relevant to the solution of the problem at hand. This may be in the form of a direct result yielding a numerical value,[16] or one may have a statistical result, in which a sufficient number of measurements must be repeated to obtain an average quantity with sufficient accuracy.[17]

To motivate the utility of nonlinear transformations in quantum computing, consider the problem of searching through all possible ways of completing a task, to find an optimal one. The number k will represent one of the possible pathways, and we will assume that the binary representation of this number (i.e. values of the qubits) can be grouped into successive "moves" or "choices" which must be carried out to follow this pathway. For example, consider the following qubit decomposition of the state $|k\rangle$:

$$|k\rangle = \left|\underbrace{q_1 q_2 \cdots q_m}_{\text{move 1}} \underbrace{q_{m+1} \cdots q_{2m}}_{\text{move 2}} \underbrace{q_{2m+1} \cdots q_{3m}}_{\text{move 3}} \cdots \right\rangle . \tag{4}$$

This would correspond to labeling all possible pathways which could be reached by a finite number of discrete moves to be chosen from a finite number of possibilities. For example, for the traveling salesman problem[18] with 256 cities, one could assign consecutive $m = 8$ qubits to represent the city to be visited at that stage, and one would need 256 such 8-qubits to represent the complete trip. (Obviously, this procedure would also produce some pathways which are "illegal" in the way this problem is defined, but these will be discarded in the solution.) Alternatively, if the remaining consecutive steps in an ongoing chess game were to be described by $|k\rangle$, then one could use 12 consecutive qubits to describe motion of a piece from a general point on the 8×8 square to another point on the square. All possible games with a total of 100 moves could be represented by a total of 12×100 qubits. (Again, this type of coding generates an overwhelming ratio of illegal moves, which need to be discarded.) The function $|f(k)\rangle$ is arranged to hold information about the end result of the decision process, for example, whether the completed moves correspond to a "legal" sequence, and if so, what the result is. The "result" here would be whether the game has been "won" or, what the total distance traveled is within the context of the traveling salesman problem mentioned above.

Note that the superposed state may be factored so that it can be expressed as a sum over the more significant qubits representing the number k, multiplying the two terms corresponding to the least significant qubit:

$$\frac{1}{\sqrt{N}} \sum_{j=0}^{N/2-1} |j\rangle(|0\rangle|f(j|0)\rangle + |1\rangle|f(j|1)\rangle)\,, \tag{5}$$

where the notation $(j|0) = 2j$ and $(j|1) = 2j+1$ has been used. Note that for each j, there is a "preferred" choice between the cases $(j|0)$ and $(j|1)$ (based on the values of $f(j|0)$ and $f(j|1)$), which we will label as j'. One could then obtain a superposed state with a reduced number of terms if the following transformation could be made:

$$\frac{1}{\sqrt{2}}(|0\rangle|f(j|0)\rangle + |1\rangle|f(j|1)\rangle) \to |f(j')\rangle\,, \tag{6}$$

so that the new state is

$$\frac{1}{\sqrt{N/2}} \sum_{j=0}^{N/2-1} |j\rangle|f(j')\rangle\,. \tag{7}$$

This process could then be iterated until a single qubit remains, yielding its optimal value. Once this value is determined, the problem is reduced to the determination of the remaining $N-1$ qubits, for which the above process must be repeated, starting with these $N-1$ qubits. The number of operations necessary for the determination of all of the qubits then can be seen to be proportional to N^2, one factor of N coming from the repetition of the operation for each qubit to be determined, and another factor from the number of transformations of the type shown in Eq. (6).

For many problems of interest however, including the ones mentioned above as examples, this transformation cannot be achieved with unitary operations. Nonlinearity allows for "communication" between pairs of superposed states in carrying out the operation in Eq. (6). For example, the simple logical NOR operation (which is related to how the "legality" operation of the moves would transform) would need to have

$$\frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|0\rangle) \to |1\rangle\,, \tag{8}$$

$$\frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle) \to |0\rangle\,, \tag{9}$$

$$\frac{1}{\sqrt{2}}(|0\rangle|1\rangle + |1\rangle|0\rangle) \to |0\rangle\,, \tag{10}$$

$$\frac{1}{\sqrt{2}}(|0\rangle|1\rangle + |1\rangle|1\rangle) \to |0\rangle\,. \tag{11}$$

The operation is clearly nonlinear, as Eqs. (8)–(11) above demonstrate: The sum of the left sides of Eqs. (8) and (11) of the transformation equals the sums of the left hand sides of Eqs. (9) and (10), but the same obviously is not true for the right hand sides.

A similar discussion may be carried out for optimization problems of the traveling salesman type, obtaining an optimal set of "moves" by the pairwise elimination of non-preferred choices. Details cannot be provided here, but it has to be remembered that the standard tools of classical logical computation (such as the logical AND and OR operations) may be utilized if nonlinear transformations are to be allowed. This feature then (at least in principle) makes accessible to quantum computation all classical problems which can benefit from parallelism.

3. Nonlinear Schrödinger Equation

The transformation in Eqs. (8)–(11) may be implemented as the result of time-development through a nonlinear Hamiltonian. As an example, we will consider a Hamiltonian of the Gross–Pitaevskii type[19–21] in which an extra potential term proportional to the square magnitude of the wavefunction appears. The two-qubit state $|q_0 q_1\rangle$ with q_0 and q_1 equal to 0 or 1 will be taken to be related to the occupation of four sites at $\mathbf{r}(q_0, q_1) = (q_0\hat{\imath} + q_1\hat{\jmath})\Delta x$ where $\hat{\imath}$ and $\hat{\jmath}$ are the unit vectors in the x and y directions respectively. The system then corresponds to a set of four quantum sites arranged as a square with side Δx. The Schrödinger equation describing the system will then be

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi(q_0, q_1) = &-\frac{\hbar^2}{2m(\Delta x)^2}\left[\psi(\bar{q_0}, q_1) + \psi(q_0, \bar{q_1}) - 2\psi(q_0, q_1)\right] \\ &+ [V(q_0, q_1) + \alpha|\psi(q_0, q_1)|^2]\psi(q_0, q_1)\,, \end{aligned} \tag{12}$$

where α is a measure of the nonlinearity in the system, and we have used the shorthand notations $\bar{q} = 1 - q$ and $\psi(q_0, q_1) = \psi(\mathbf{r}(q_0, q_1))$. The first term on the right hand side is the kinetic energy term of the square geometry. It may also result through a tight-binding interpretation of the interaction among four quantum wells. The coefficient of this term $\epsilon = \hbar^2/2m(\Delta x)^2$ with energy units, sets the physical scales of the system. The external potential V is the quantity to be "engineered" so that the time-development of ψ has the required form.

Figure 1 shows the occupation probabilities of the four sites in the system as a function of time, for the initial conditions indicated in Eqs. (8)–(11). Note that for the choice of the potential values corresponding to this figure, the value of the $\psi(1, 1)$ component of the state vector yields deterministically (i.e. with magnitude either zero or one) the corresponding states at the right hand side of Eqs. (8)–(11).

The numerical computation was performed for values of the unitless time parameter $\tau = t\epsilon/\hbar$ between 0 and 7.665, $\alpha/\epsilon = 2.350$, and the four values of the potential $V(0, 0) = -0.003554\epsilon$, $V(0, 1) = 2.124\epsilon$, $V(1, 0) = 2.352\epsilon$, and $V(1, 1) = 0$. The numerical integration of the Schrödinger equation was carried out by

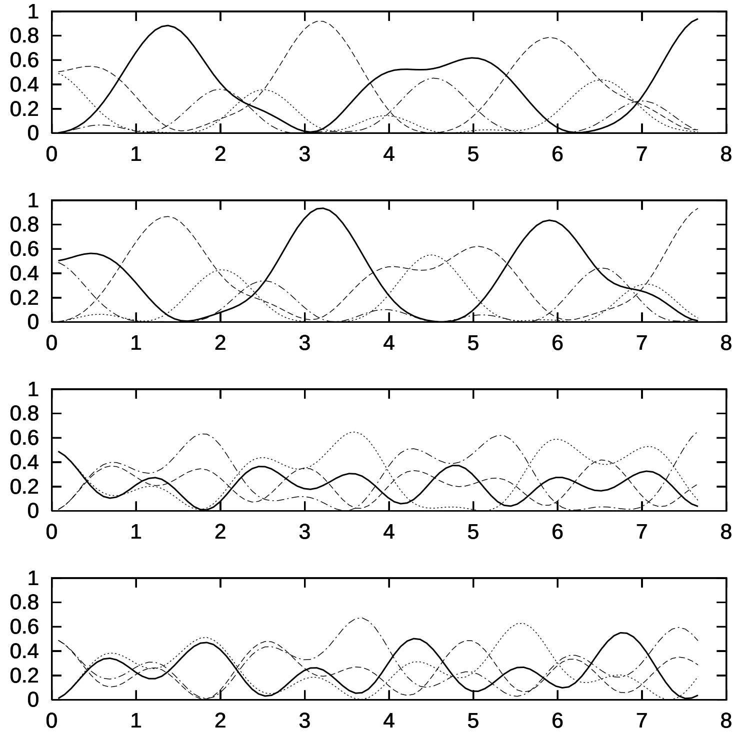

Fig. 1. The squared magnitudes of $\psi(0,0)$ (dashed lines), $\psi(0,1)$ (dotted lines), $\psi(1,0)$ (dot-dashed lines), and $\psi(1,1)$ (thick continuous lines) for four different initial conditions. The initial conditions correspond to the left hand terms of expressions 8 through 11 from top to down respectively. Parameters of the numerical computation are given in the text. Note that the final value of square magnitude of $\psi(1,1)$ correlates with the right hand terms of expressions 8 through 11.

factorizing the kinetic and potential energy terms in the exponential and treating each part exactly.[22] This procedure is correct to the second order in the integration timestep, which was taken to be $\Delta\tau = 7.665 \times 10^{-4}$. The four final values of $\psi(1,1)$ are within 0.06, 0.01, 0.04, and 0.04 of their ideal values. Other solutions to the problem could be found. One needs to adjust the values of α, τ, and the three finite values of the potential until the final value of $\psi(1,1)$ is within acceptable error. (The fourth value of the potential is the arbitrary reference of the potential energy and was chosen as zero.) The aim at this stage was not to obtain a solution with overwhelming accuracy to an idealized model but to show that nonlinear quantum transformations are available. A physical realization of such a functional block would necessarily be more complicated and would require a more careful analysis.

The implementation of the nonlinear qubit transformation then involves the teleportation of the two initial qubits into the wavefunction ψ, and the teleportation of a single qubit of information out of $\psi(1,1)$ after a fixed period of time.

4. Conclusions

In conclusion, we have shown that evolution of a quantum system with dynamics controlled by a nonlinear Schrödinger equation enables nonlinear transformations to be carried out on qubits, which may be used to implement quantum computational algorithms with less restrictions. It may also be possible to use the nonlinearity to "saturate" the qubits to some ideal values close to their initial states, thereby implementing some error correction. (Quantum state purification through the use of nonlinear transformations has been discussed in Ref. 23.)

It is also evident the development of the quantum system and its measurements yield continuous values, and that the discussion in this paper may also be relevant to introducing nonlinearities to continuous-variable quantum computation.[24–26]

A question that needs to be considered at this point is whether the nonlinear time development is that of a true quantum system, as microscopic interactions always lead to unitary development. The assumptions that go into the development of the approximations that lead to the nonlinear Schrödinger equation may limit the applicability of the corresponding dynamics to the description of wave phenomena without the quantum features (such as the second sound effect in superfluid helium). It needs to be confirmed that the degrees of freedom described by this equation still maintains the indispensable quantum properties of interference, entanglement, and the probability interpretation, and is not just a collective macroscopic wave phenomena. Experimental work studying the interference effects in BEC systems[27,28] and the detailed theoretical analysis of their entanglement[12] seem to indicate that the Gross–Pitaevskii equation may indeed be valid in representing genuine quantum effects in these systems.[29] Perhaps another way of looking at this validity is to interpret these transformations as high fidelity representations of nonlinearities through the use of the large number of quantum background degrees of freedom (individually obeying unitary time development) contained in the "mean field" of the system.

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