Nonresonant effects in the implementation of the quantum Shor algorithm

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We simulate Shor's algorithm using the Ising spin quantum computer. The influence of nonresonant effects is analyzed in detail. It is shown that the method developed earlier in our papers successfully suppresses nonresonant effects even for relatively large values of the Rabi frequency.

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I. QUANTUM SHOR ALGORITHM

The quantum Shor algorithm [1] provides an exciting opportunity for prime factorization of large integers—a problem beyond the capabilities of today's powerful digital computers. Shor's algorithm utilizes two quantum registers (the x and y registers), which contain two-level quantum systems called qubits [1–3]. First, the quantum computer produces the uniform superposition of all states in the x register—all possible values of x. Second, the quantum computer computes the periodic function $y(x) = q^x \pmod{N}$, where N is the number to factorize, and q is any number that is coprime to N. Third, the quantum computer creates a discrete Fourier transform of the x register. Measurement of the state of the x register yields the period T of the function y(x), which is used to produce a factor of the number N.

In Dirac notation, the wave function of the quantum computer can be represented as a superposition of digital states,

$$|a_{L-1}a_{L-2}\cdots a_1a_0,b_{M-1}b_{M-2}\cdots b_1b_0\rangle,$$
 (1)

where a_k ($0 \le k \le L-1$) denotes the state of the kth qubit in the x register, and b_n ($0 \le n \le M-1$) denotes the state of the nth qubit in the y register. For example, if the kth qubit of the x register is in the ground state, then $a_k = 0$, and if it is in the excited state, $a_k = 1$.

In decimal notation, the digital state can be represented as $|x,y\rangle$, where

$$x = \sum_{k=0}^{L-1} a_k 2^k, \quad y = \sum_{n=0}^{M-1} b_n 2^n.$$
 (2)

In this notation, the initial wave function of a quantum system is $|0, 0\rangle$. A uniform superposition of the states created in the *x* register can be written as

$$\Psi = \frac{1}{\sqrt{D}} \sum_{x} |x,0\rangle, \tag{3}$$

where $D = 2^L$ is the number of states in the x register. After computation of the function y(x), we have

$$\Psi = \frac{1}{\sqrt{D}} \sum_{x} |x, y(x)\rangle. \tag{4}$$

After discrete Fourier transform, one measures the state of the x register. The probability of the measurement, P(x), must be a peaked distribution with peak separation Δx equal to a multiple of 1/T. In particular, if the number of states D in the x register is divisible by the period T, then $\Delta x = D/T$. From the value Δx one can find the period T. A factor of the number N can be found by computing the greatest common divisor of $(q^{T/2}+1)$ and N, or $(q^{T/2}-1)$ and N (for even T).

It was shown in [4] that the simplest demonstration of the quantum Shor algorithm can be done with only four qubits. (Two qubits represent the x register and two qubits represent the y register.) This primitive quantum computer is able to find a factor of the number 4. For N=4, the only coprime number is q=3. The function $y(x)=3^x \pmod{4}$, has only two values, y=1 and y=3, and the period is T=2. In Dirac notation, the wave function (4) has the form

$$\Psi = \frac{1}{2}(|00,01\rangle + |01,11\rangle + |10,01\rangle + |11,11\rangle). \tag{5}$$

After discrete Fourier transform, the wave function of the quantum computer is

$$\Psi = \frac{1}{2}(|00,01\rangle + |00,11\rangle + |10,01\rangle + |10,11\rangle). \tag{6}$$

Measuring x can produce two values: x=0 and x=2. So $\Delta x=2$, and the period is $P=D/\Delta x=2$. Finally, $q^{P/2}-1=3-1=2$, and the factor of 4 can be found as the greatest common divisor of 4 and 2.

II. ISING SPIN QUANTUM COMPUTER

The Ising spin quantum computer, first introduced in [5], consists of a one-dimensional chain of 1/2 spins, connected by Ising interactions. The quantum logic gates can be implemented in the Ising spin quantum computer using selective electromagnetic pulses which induce transitions between the ground state and the excited state of a chosen spin. The Hamiltonian of the quantum computer during the action of the nth electromagnetic pulse can be written as

$$\mathcal{H} = -\sum_{k=0}^{S-1} \left[\omega_k I_k^z + \frac{1}{2} \Omega_{kn} (e^{-i(\omega^n t + \varphi_n)} I_k^- + e^{i(\omega^n t + \varphi_n)} I_k^+) \right]$$

$$-2\sum_{k=0}^{S-2} J_{k,k+1} I_k^z I_{k+1}^z, \tag{7}$$

where ω_k is the resonant frequency of the kth spin; Ω_{kn} is the Rabi frequency of the kth spin during the nth pulse; ω^n and φ_n are the frequency and the phase of the nth electromagnetic pulse; $J_{k,k+1}$ is the constant of the Ising interaction; I_k^z and $I_k^{\pm} = I_k^x \pm iI_k^y$ are the operators for the kth 1/2 spin; S is the total number of spins (qubits) in the quantum computer; and we choose units in which $\hbar = 1$. A difference of resonant frequencies between spins (qubits) can be provided by differences in the gyromagnetic ratio of the spins or by a nonuniform external magnetic field. The Ising interactions also influence the resonant frequency, providing an opportunity for conditional logic gates. The main disadvantage of the Ising spin quantum computer is the presence of nonresonant effects: a selective electromagnetic pulse that is resonant to a specific spin influences all other spins of the quantum computer.

Destructive nonresonant effects can be significantly weakened by using a $2\pi k$ method suggested in [6] (see also [3], Chap. 22). The main idea of this method is that parameters of the electromagnetic pulse should be chosen in such a way that a nonresonant spin rotates about the effective magnetic field by an angle of $2\pi k$ (where k is an integer). So, at the end of the pulse, it returns to its initial position.

To the best of our knowledge, this paper provides the first simulation of the quantum Shor algorithm, taking into consideration nonresonant effects. We investigate the destructive influence of nonresonant effects and show that one can significantly reduce nonresonant effects by using $2\pi k$ pulses.

III. SIMULATION OF QUANTUM COMPUTATION

We describe the four-qubit quantum computer with the Hamiltonian (7) putting S=4, $\omega_{k+1}=\omega_k+\Delta\omega$, $\Omega_{kn}=\Omega$, and $J_{k,k+1}=J$. We count spins (qubits) from the right to the left. The values of the parameters will be given below. To implement the Shor algorithm we consider application of 16 selected resonant pulses. The Hamiltonian (7) suggests that the nth pulse is "cut" from a continuous harmonic oscillation $\exp(i\omega^n t)$ and its phase is shifted by φ_n . For example, the first pulse has frequency $\omega^1=\omega_2+2J$ and phase $\varphi_1=\pi/2$; the second pulse has frequency $\omega^2=\omega_3+J$ and phase $\varphi_2=\pi/2$, and so on. We will use single-integer decimal notation for the four-spin basic states, i.e.,

$$|p_3p_2,p_1p_0\rangle = |p\rangle$$
, $p = p_0 + 2p_1 + 2^2p_2 + 2^3p_3$,

and c_p is the amplitude corresponding to the state $|p\rangle$. The Schrödinger equation for the amplitude c_p of the state $|p\rangle$ can be written as

$$i\dot{c}_{p} = \sum_{m=0, m \neq p}^{15} c_{m}V_{pm} \exp[i(E_{p} - E_{m})t + r_{pm}(\omega^{n}t + \varphi_{n})].$$
 (8)

Here we use the interaction representation, i.e., $c_p \rightarrow c_p \exp(-iE_p t)$; V_{pm} is the matrix element between the states $|p\rangle$ and $|m\rangle$, which is equal to $V_{pm} = -\Omega/2$ for single-spin transitions and zero for other transitions; E_p and E_m are the energies of the corresponding states, $r_{pm} = -1$ for E_p

 $>E_m$, and $r_{pm}=1$ for $E_p < E_m$. If one neglects nonresonant effects, the *n*th pulse produces only a rotation of a resonant spin, which can be described as a transformation of the basic states:

$$|0\rangle \rightarrow \cos(\alpha_n/2)|0\rangle + i\exp(-i\varphi_n)\sin(\alpha_n/2)|1\rangle,$$

$$|1\rangle \rightarrow \cos(\alpha_n/2)|1\rangle + i\exp(i\varphi_n)\sin(\alpha_n/2)|0\rangle,$$
(9)

where $\alpha_n = \Omega \tau_n$ is the angle of rotation of the average spin and τ_n is the duration of the *n*th pulse. For example, the first two pulses are the $\pi/2$ pulses, i.e., $\alpha_1 = \alpha_2 = \pi/2$.

Instead of a direct discrete Fourier transform we have used an idea of Coppersmith and Deutsch, first described in [7]. Following this idea, the final wave function (without nonresonant effects) contains four states:

$$|00,01\rangle, |00,11\rangle, |01,01\rangle, |01,11\rangle.$$
 (10)

One must reverse the results of the measurement of the x register to get the actual result of the discrete Fourier transform. Following this rule, one obtains x=0 and x=2 with equal probability, 1/2.

It follows from (10) that in the resonant approximation we have

$$|c_1|^2 = |c_3|^2 = |c_5|^2 = |c_7|^2 = 1/4,$$
 (11)

and zero probabilities for all other states.

IV. RESULTS OF SIMULATIONS OF THE SHOR ALGORITHM

Figure 1(a) shows the actual values of the "resonant" probabilities (11) for the following values of the parameters:

$$\Delta \omega = 10, J = 1, \Omega = 0.1.$$
 (12)

(All parameters are dimensionless and are measured in units of J.) One can see that the expression (11) is approximately satisfied. Small deviations of the resonant probabilities from 1/4 are associated with nonzero probabilities for "nonresonant" states. Figure 1(b) (with a magnified scale) shows that nonresonant states are very nonuniformly excited: the probability of the highest state $|15\rangle$ is close to 10^{-3} ; the probabilities of the states $|9\rangle$ and $|11\rangle$ are close to 10^{-4} ; and all other nonresonant probabilities have smaller values. Figure 2 shows a radical change of the results for a small increase of the Rabi frequency (from Ω =0.1 to Ω =0.112). Now the probabilities of the resonant states are significantly different: the probability of measuring x=2 is noticeably greater than for the value x=0. The probability of error connected with nonresonant states has sharply increased.

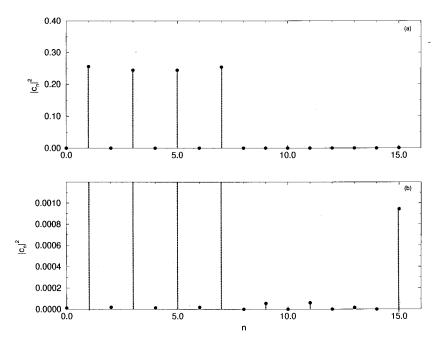


FIG. 1. Probabilities of the states $|n\rangle,|c_n|^2$ $(n=0,\ldots,15)$ at the end of the Shor algorithm. The parameters are $\Delta\omega=10$, J=1.0, and $\Omega=0.1$. (a) The probabilities for the "resonant" states, with complex amplitudes c_1 , c_3 , c_5 , and c_7 ; (b) the probabilities for other states (which remain small), at different scale.

dence of resonant probabilities on the value of the Rabi frequency Ω , which continuously approaches the value of the Ising constant J. The resonant probabilities are close to Eq. (11) at fixed values of Ω :

$$\Omega = 0.1, 0.125, 0.1666, 0.25.$$
 (13)

The last point where the probabilities approach the value 1/4 is $\Omega = 0.51639$, but the deviation from 1/4 at this point is much greater than for previous values of Ω [Eq. (13)]. Figure 5 demonstrates the destruction of the Shor algorithm when the value of the frequency difference between neighboring qubits, $\Delta \omega$, approaches the value of the Ising constant J. [The Rabi frequency Ω and J are given by Eq. (12).] Significant deviation of the probabilities from their "resonant" val-

ues begins at approximately $\Delta \omega = 3$. The greatest probability of error occurs in the highest state, $|15\rangle$. Figure 6 shows the time dependence of the resonant probability $|c_3|^2$ during the action of the last two pulses, for different values of $\Delta \omega$. One can see that for $\Delta \omega \ge 4$, the function $|c_3(t)|^2$ is approximately independent of $\Delta \omega$. For $\Delta \omega \le 3$, this function depends significantly on $\Delta \omega$.

Note that, in Figs. 1–6, the angles of rotation α_n did not change, i.e., the increase of Ω was compensated by decrease of the pulse duration τ_n . Figure 7 shows the destruction of Shor's algorithm when the phases φ_n deviate randomly from their correct values φ_n^0 . The phases were chosen randomly in the interval $(\varphi_n^0 - \varepsilon, \varphi_n^0 + \varepsilon)$, for four values of ε . Significant influence of the phase fluctuations can be observed at $\varepsilon \ge 0.5$ rad. Again, the main error occurs in the highest state,

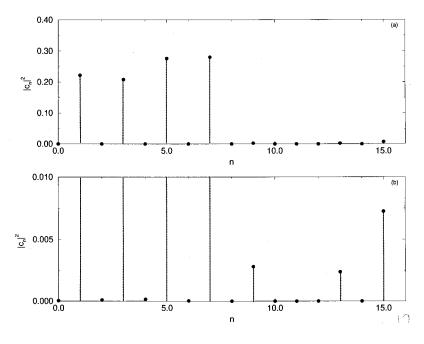


FIG. 2. The same as in Fig. 1, for $\Omega = 0.112$.

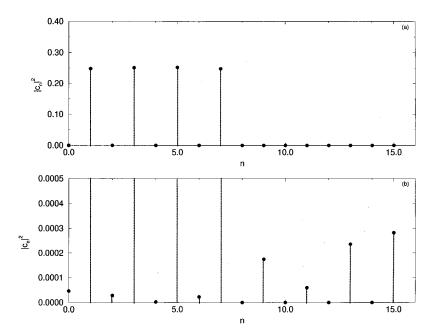


FIG. 3. The same as in Fig. 1, for $\Omega = 0.125$.

|15\). Figure 8 shows the influence of the fluctuation of the angle of rotation α_n on the performance of Shor's algorithm. We have randomly changed the values of τ_n in the interval $(\tau_n^0 - \varepsilon, \tau_n^0 + \varepsilon)$, for different values of ε . The values of Ω , $\Delta \omega$, and τ_n^0 are given by Eq. (12), where τ_n^0 is the correct value of τ_n . A noticeable destruction in the performance of Shor's algorithm was observed at $\varepsilon \ge 2$. The corresponding angle of rotation is $\Omega \varepsilon \ge 0.2$ rad.

V. DISCUSSION

The most important result of our simulation of Shor's algorithm is the successful periodic suppression of nonresonant effects when the value of the Rabi frequency Ω approaches the Ising constant J. We shall now discuss this phenomenon in detail.

Suppose the *n*th electromagnetic pulse induces a nonresonant transition between the states $|p\rangle$ and $|m\rangle$, where $E_p > E_m$. The equation of motion (8) for these two states can be written approximately as

$$\begin{split} i\dot{c}_p &= -(\Omega/2)c_m \exp\{i[(E_p - E_m - \omega^n)t - \varphi_n]\},\\ i\dot{c}_m &= -(\Omega/2)c_p \exp\{i[(E_m - E_p + \omega^n)t + \varphi_n]\}. \end{split} \tag{14}$$

Here we assume that the probability of a nonresonant transition between the states $|p\rangle$ and $|m\rangle$ is much greater than any other transition probability involving these two states. With an accuracy up to the phase, the solution of Eq. (14) can be written as

$$c_p(t_n) = c_p(t_{n-1}) \left[\cos(\Omega_e \tau_n/2) - (i\Delta/\Omega_e) \sin(\Omega_e \tau_n/2) \right]$$

$$+ c_m(t_{n-1}) \left[(i\Omega/\Omega_e) \sin(\Omega_e \tau_n/2) \right], \qquad (14a)$$

$$\begin{split} c_m(t_n) &= c_m(t_{n-1}) \big[\cos(\Omega_e \tau_n/2) + (i\Delta/\Omega_e) \sin(\Omega_e \tau_n/2) \big] \\ &+ c_p(t_{n-1}) \big[(i\Omega/\Omega_e) \sin(\Omega_e \tau_n/2) \big]. \end{split}$$

Here Ω_e is the effective frequency for the nonresonant transition,

$$\Omega_{\rho} = (\Omega^2 + \Delta^2)^{1/2},\tag{15}$$

and $\Delta = E_p - E_m - \omega^n$. (t_{n-1}, t_n) is the time interval of the *n*th pulse; $t_n - t_{n-1} = \tau_n$.

One can see that for $\Omega_e \tau_n = 2 \pi k$ (k = 1, 2, ...) the probability of nonresonant transitions vanishes. This is the main idea of the " $2 \pi k$ " method [3,6]. For a π pulse ($\Omega \tau_n = \pi$), the values of Ω that satisfy this $2 \pi k$ condition are

$$\Omega = |\Delta|/\sqrt{4k^2 - 1} = |\Delta|/\sqrt{3}, |\Delta|/\sqrt{15}, |\Delta|/\sqrt{35}, |\Delta|/\sqrt{63}, \dots$$
(16)

For a $\pi/2$ pulse, the corresponding values of Ω are

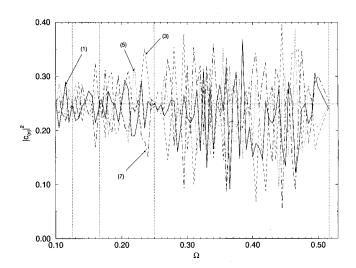


FIG. 4. Probabilities $|c_1|^2$, $|c_3|^2$, $|c_5|^2$, and $|c_7|^2$ at the end of the Shor algorithm, as a function of the Rabi frequency Ω . The parameters are $\Delta \omega = 10$ and J = 1.0.

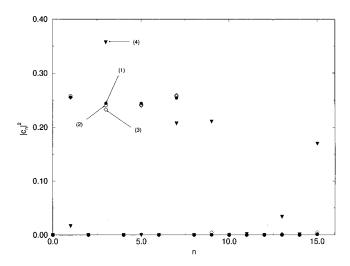


FIG. 5. Probabilities $|c_n|^2$ $(n=0,\ldots,15)$ at the end of the Shor algorithm, for different values of $\Delta\omega$: (1) $\Delta\omega=10$; (2) $\Delta\omega=6$; (3) $\Delta\omega=4$; (4) $\Delta\omega=3$. The parameters are $\Omega=0.1$ and J=1.0.

$$\Omega = |\Delta| / \sqrt{16k^2 - 1} = |\Delta| / \sqrt{15}, |\Delta| / \sqrt{63}, \dots$$
 (17)

If the Rabi frequency satisfies the $2\pi k$ condition (17) for a $\pi/2$ pulse, it automatically satisfies the condition (16) for a π pulse.

Let us consider the most probable nonresonant transitions in our system. We assume that $J{\leq}\Delta\omega$, so the most probable nonresonant transitions occur when the frequency difference $|\Delta|$ is of the order of J. For the right spin (k=0) and the left spin (k=3) we have two frequencies depending on the state of the only neighbor: $\omega_k + J$ and $\omega_k - J$. If the rf pulse is turned on either of these transitions, the frequency difference $|\Delta|$ for the other one will be 2J. For the inner spins (k=1,2), we have three possible resonant frequencies: ω_k ,

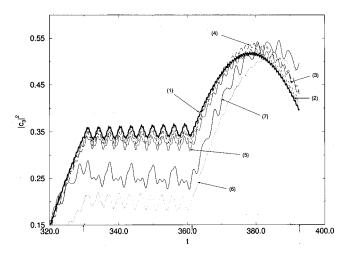


FIG. 6. Dynamics of the probability $|c_3(t)|^2$ near the end of the Shor algorithm, for different values of $\Delta\omega$: (1) $\Delta\omega=10$; (2) $\Delta\omega=8$; (3) $\Delta\omega=6$; (4) $\Delta\omega=5$; (5) $\Delta\omega=4$; (6) $\Delta\omega=3$; (7) $\Delta\omega=2$. The parameters are J=1 and $\Omega=0.1$. Arrows show the end of the 14th, 15th, and 16th pulses.

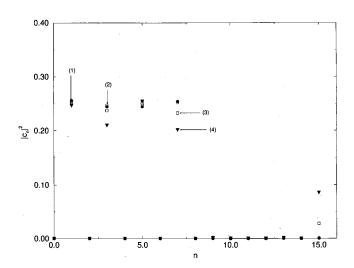


FIG. 7. Probabilities $|c_n|^2$ $(n=0,\ldots,15)$ at the end of the Shor algorithm, for random phases $\varphi_k = \varphi_k^{(0)} + \Delta \varphi_k$; $\varphi_k^{(0)}$ are the required phases of the pulses $(k=1,\ldots,16)$; $\Delta \varphi_k$ are random phases chosen in the interval $\Delta \varphi \in [-\epsilon,\epsilon]$. (1) $\epsilon = 0$, (2) $\epsilon = 0.1$, (3) $\epsilon = 0.5$, (4) $\epsilon = 0.8$. The parameters are $\Delta \omega = 10$, $\Omega = 0.1$, and J = 1.0.

 $\omega_k - 2J$, and $\omega_k + 2J$. The frequency difference $|\Delta|$ can take two values: 2J and 4J.

One cannot suppress both nonresonant transitions with $|\Delta| = 2J$ and $|\Delta| = 4J$. Putting $|\Delta| = 2J$ in Eq. (17) we obtain

$$\Omega = 2J/\sqrt{16k^2 - 1} \approx J/2k.$$

For $|\Delta| = 4J$, we have

$$\Omega = 4J/\sqrt{16k^2-1} \approx J/k$$
.

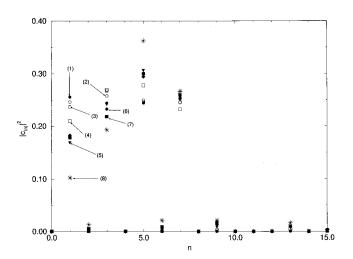


FIG. 8. Probabilities $|c_n|^2$ $(n=0,\ldots,15)$ at the end of the Shor algorithm, for random duration of resonant pulses τ_n $(n=1,\ldots,16);\ \tau_n=\tau_n^{(0)}+\Delta\tau_n$, where $\tau_n^{(0)}$ is the required duration of the nth pulse, and $\Delta\tau_n$ is a random variable uniformly distributed between $-\epsilon$ and $+\epsilon$. (1) $\epsilon=0$; (2) $\epsilon=0.5$; (3) $\epsilon=1$; (4) $\epsilon=2$; (5) $\epsilon=3$; (6) $\epsilon=4$; (7) $\epsilon=5$; (8) $\epsilon=7$. The parameters are $\Delta\omega=10$, $\Omega=0.1$, and J=1.0.

So, if one satisfies the $2\pi k$ condition for $|\Delta|=2J$, one satisfies approximately the same condition for $|\Delta|=4J$. But total suppression of two nonresonant transitions is impossible.

Now we consider an example—the suppression of nonresonant effects during the first two pulses. The initial state of our system is the ground state, $|00,00\rangle$. First, we apply a $\pi/2$ pulse with the frequency ω_2+2J , which is resonant with the spin with number k=2. The nonresonant effects for three other spins are small if $\Delta\omega$ is large enough. After the action of the first pulse, we have the superposition

$$(1/\sqrt{2})(|00,00\rangle + |01,00\rangle).$$
 (18)

Next, we apply a $\pi/2$ pulse with the frequency $\omega_3 + J$. This pulse is resonant with the k=3 spin [in the ground state, the first term in Eq. (18)]. But this pulse also perturbs the same spin in the excited state [the second term in Eq. (18)]. The frequency of the transition for the spin with k=3 in the second term in Eq. (18) is $\omega_3 - J$. So the frequency difference is $|\Delta| = 2J$. Taking a value of Ω that satisfies Eq. (17) with $|\Delta| = 2J$, one suppresses this nonresonant transition.

Putting $\Omega = 2J/\sqrt{16k^2 - 1}$ with J = 1 we obtain the values

$$\Omega \approx 0.100, 0.125, 0.167, 0.252, 0.516,$$

which are close to the values obtained from computer simulations.

To decrease the time of quantum computation, one should use the largest possible values of Ω . If the acceptable probability of error state is of the order of 10^{-3} , then one should use the value $\Omega \approx 0.25$. If a probability of the error state of 10^{-2} is acceptable, one can use the value $\Omega \approx 0.516$. The time of quantum computation can be further reduced if one uses different values of Ω for $\pi/2$ and π pulses. According to Eqs. (16) and (17), the maximum value of the Rabi frequency Ω for a 2π rotation of nonresonant spins is Ω ≈ 0.51639 for $\pi/2$ pulses, and $\Omega \approx 1.1547$ for π pulses. Figure 9 shows the probabilities of the states for this minimaltime Shor's algorithm implementation. The greatest probability of error $\sim 10^{-2}$ is connected with the states $|11\rangle$ and $|15\rangle$. Note that for π pulses the value of the Rabi frequency is greater than J and the $2\pi k$ method still suppresses the nonresonant effects.

VI. CONCLUSION

We reported a simulation of the quantum Shor algorithm for prime factorization taking into consideration nonresonant effects. We have considered the Ising spin quantum computer of four qubits: two qubits in the x register, and two qubits in the y register. This primitive quantum computer is able to factor the smallest composite number, N=4. While a simulation of a much more complicated system of 15 qubits was reported in [8], that work deals with well-separated ions in an ion trap and it does not take into consideration nonresonant effects.

We have studied the destructive influence of nonresonant effects when the Rabi frequency Ω approaches the value of the Ising interaction constant J. We also studied the influence

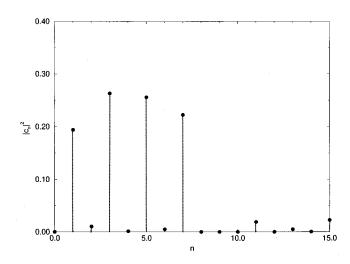


FIG. 9. Probabilities $|c_n|^2$ $(n=0,\ldots,15)$ at the end of the Shor algorithm, for four qubits. The parameters are $\Delta \omega = 10$, J = 1.0, $\Omega = 2/\sqrt{3}$ for π pulses, and $\Omega = 2/\sqrt{15}$ for $\pi/2$ pulses.

of random fluctuations of the duration and phase of the electromagnetic pulses.

The main results of our consideration are as follows.

(1) When the Rabi frequency Ω approaches the Ising interaction constant J, there is no monotonic increase of destructive nonresonant effects. Nonresonant effects are suppressed effectively when the value of Ω satisfies

$$\Omega = 2J/\sqrt{16k^2 - 1}, \quad k = 1, 2, \quad .$$
 (19)

for all pulses. These values correspond to a $2\pi k$ rotation of the nonresonant spin whose frequency is the closest to the resonant frequency. This method of suppression of nonresonant effects $(2\pi k \text{ method})$ was suggested in [6] and discussed in [3,4,9]. But this method has never been verified for a quantum computer algorithm.

- (2) The $2\pi k$ method allows one to decrease the total time of computation by taking the maximum possible value of Ω . The minimum time of computation was achieved at the values $\Omega = 2J/\sqrt{15}$ for $\pi/2$ pulses, and $\Omega = 2J/\sqrt{3}$ for π pulses. The probability of measuring an error state at these values of Ω was of the order 10^{-2} (Fig. 9).
- (3) The probability of error caused by nonresonant effects or by random fluctuation of parameters is connected with a relatively small number of states. As a rule, one, two, or three error states have a probability of excitation much greater than all other error states taken together. Normally, the highest state has a large probability of excitation.

The next step should include a bigger number of qubits, and application of the $2\pi k$ method together with error correction approaches.

ACKNOWLEDGMENTS

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