

## Decoherence in Ion Trap Quantum Computers

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(Received 28 March 1996)

The *intrinsic* decoherence from vibrational coupling of the ions in the Cirac-Zoller quantum computer [Phys. Rev. Lett. **74**, 4091 (1995)] is considered. Starting from a state in which the vibrational modes are at a temperature  $T$ , and each ion is in a superposition of an excited and a ground state, an adiabatic approximation is used to find the inclusive probability  $P(t)$  for the ions to evolve as they would without the vibrations, and for the vibrational modes to evolve into any final state. An analytic form is found for  $P(t)$  at  $T = 0$ , and the decoherence time is found for all  $T$ . The decoherence is found to be quite small, even for 1000 ions. [S0031-9007(96)00750-8]

PACS numbers: 89.80.+h, 03.65.Db, 32.80.Pj, 36.40.-c

Quantum computers (QC) are (as yet hypothetical) devices with states that are quantal in nature, and which perform calculations by unitary transformations on these states [1–3]. The linearity of the superposition principle leads to an in-built massive parallelism: a computer with  $N$  two-state elements can operate on  $2^N$  states simultaneously. This parallelism underlies Shor's recent algorithm [4] for factorizing a composite number of order  $2^L$  in  $\sim L^3$  steps on a QC. The best known classical algorithm takes  $\sim \exp[c(L)L^{1/3}]$  steps with  $c(L) \sim (\ln L)^{2/3}$ . The potential for other quantum algorithms is clearly exciting, as is the emergence of a new paradigm for computation itself.

It is obvious that maintaining perfect phase coherence among all the states of a QC is a daunting task, not to mention getting these states to evolve in the desired fashion in the first place [5]. An imaginative proposal for a QC by Cirac and Zoller (CZ) [6] seems promising in addressing these problems [7,8]. It utilizes a string of  $N$  identical ions in a linear Paul trap [9], with each ion separately addressable by a laser. Two internal states of each ion,  $|e\rangle$  and  $|g\rangle$ , are used for the QC, along with the center-of-mass (CM) axial vibrational mode of the entire array. A program is implemented as a specified sequence of ( $\pi/2$ ,  $\pi$ , etc.) pulses that drive  $|e\rangle \leftrightarrow |g\rangle$  transitions on any given ion, along with pulses detuned by the CM frequency that enable coupled transitions between any pair of ions.

Two types of decoherence should be distinguished in the CZ (indeed, any) QC. The first is technical, due, e.g., to imperfect phase locking, mistuning of lasers, errors in timing and duration of pulses, and overlooked perturbations in the Hamiltonian. The second kind is intrinsic, and arises from coupling of the computationally useful to the undesirable bath degrees of freedom. Although the technical problems alone render the pursuit of a QC a fool's quest in many people's eyes, intrinsic decoherence sets basic limits on the capabilities of a QC. It is with this motivation that we study intrinsic decoherence in the CZ QC [10].

We take as our bath the vibrations of the ions, which we treat as undamped harmonic oscillators. Damping can be included if necessary [11]. Radiative decoherence

is accounted for very simply by demanding that any computation take less time than  $\tau_{\text{sp}}/N$ , where  $\tau_{\text{sp}}$  is the spontaneous  $|e\rangle \rightarrow |g\rangle$  decay time for one ion. It clearly pays to have as large a  $\tau_{\text{sp}}$  as possible, by working with  $E1$  forbidden transitions [6], or with hyperfine sublevels of the ground ionic multiplet [7]. The total Hamiltonian minus the driving lasers can be generally written as (setting  $\hbar = 1$ )

$$H = \frac{1}{2} \sum_i \omega_0 \sigma_{iz} + \sum_{\mu} \left( \frac{p_{\mu}^2}{2m} + \frac{1}{2} m \omega_{\mu}^2 q_{\mu}^2 \right) + \sum_{i,\mu} \sigma_{i\perp} \cdot \mathbf{c}_{i\mu} q_{\mu}. \quad (1)$$

Here, the  $\sigma$ 's are equivalent Pauli spin operators in the  $\{|e\rangle, |g\rangle\}$  space,  $\sigma_{\perp} = (\sigma_x, \sigma_y, 0)$ ,  $q_{\mu}$  and  $p_{\mu}$  are the vibrational normal mode coordinates and momenta, and  $m$  is the mass of each ion. We shall refer to the three terms in Eq. (1) as  $H_i$ ,  $H_{\text{nm}}$ , and  $H'$ , respectively. The  $\mathbf{c}_{i\mu}$  are calculable functions (see below) of the ionic transition matrix elements and equilibrium ion positions, which we assume are such that there is no  $|e\rangle \leftrightarrow |g\rangle$  transition term in  $H$  in equilibrium. It is the key to successful operation of the CZ QC that the vibrations be cooled to nearly zero temperature, and that the frequencies  $\omega_{\mu}$  and the couplings  $\mathbf{c}_{i\mu}$  be small [12]. The approximations of this paper require that  $\omega_0 \gg \omega_{\mu} \cdot \langle \sum_{\mu} \mathbf{c}_{i\mu} q_{\mu} \rangle$ , and  $\sum_{\mu} \langle \mathbf{c}_{i\mu} q_{\mu} \rangle^2 / \omega_0 \ll \omega_{\mu}$ , which as we shall see, can be satisfied comfortably.

The coupling between the ionic vibrations and the internal states of the ions will give rise to decoherence for the following reason. The vibrations create fluctuating electric fields that drive transitions between the internal states, and thus alter the time evolution of the computing degrees of freedom from that which is desired in stochastic and uncontrollable fashion. It should be noted that this decoherence is present even at zero bath temperature because of zero point ionic motion.

Let us now study the effects of the bath on the simplest computation of all, i.e., just waiting. We include the CM vibrational mode in the bath for simplicity in this note,

as this is not expected to change the result qualitatively. Suppose that initially, the bath is described by a density matrix  $\rho(Q, Q')$  ( $Q$  denotes all the  $q_\mu$  collectively), and the ions are in some state  $|\text{in}\rangle$ . The system is not driven by any lasers, and simply sits for a time  $t$ . We are interested in the probability  $P(t)$  of finding the ions in the final internal state  $|\text{fin}\rangle \equiv \exp(-iH_i t)|\text{in}\rangle$  that one would get in the absence of the bath, and the bath in any final state whatsoever. For the state  $|\text{in}\rangle$ , we take

$$|\text{in}\rangle = \prod_i 2^{-1/2}(|+\rangle_i + |-\rangle_i), \quad (2)$$

where  $\sigma_{iz}|\pm\rangle_i = \pm|\pm\rangle_i$ . This state is illustrative of the complex superpositions of computational basis states that give QC's their parallelism. Since Eq. (1) describes a finite, closed system,  $P(t) \not\rightarrow 0$  as  $t \rightarrow \infty$ , but we expect that  $P(t)$  will drop close to zero at some time  $\tau_d$ , after which it will fluctuate with small amplitude [13]. The time  $\tau_d$  limits the longest computation that can be done with the CZ QC (if  $\tau_d < \tau_{\text{sp}}/N$ ). The coherence time is expected to decrease when transitions are driven by the lasers, and can also be estimated [11].

To evaluate  $P(t)$ , we write the reduced bath density matrix propagator as a double path integral

$$J(Q_f, Q'_f; Q, Q') = \int_{Q'}^{Q_f} \int_Q^{Q'_f} [dQ][dQ'] e^{i\{S_0[Q(t)] - S_0[Q'(t)]\}} A[Q(t)] A^*[Q'(t)], \quad (3)$$

where  $S_0$  is the action for the bath alone, and

$$A[Q(t)] = \left\langle \text{fin} \left| T \exp\left(-i \int_0^t [H_i + H'(Q(t'))] dt'\right) \right| \text{in} \right\rangle. \quad (4)$$

In terms of  $J$ ,  $P(t)$  is given by

$$P(t) = \int \int \int dQ_f dQ dQ' J(Q_f, Q'_f; Q, Q') \rho(Q, Q'). \quad (5)$$

It now does no good to integrate out the oscillators. Instead, we exploit the fact that  $\omega_0 \gg \omega_\mu$ —typically  $\omega_0 \sim 10^{15} \text{ s}^{-1}$ , and  $\omega_\mu \sim 10^7 \text{ s}^{-1}$ —to integrate out *the spins*. It is easily seen that  $A[Q(t)]$  factorizes into  $\prod_i A_i[Q(t)]$ . The  $i$ th spin experiences a field  $\omega_{i\perp} = 2 \sum_\mu \mathbf{c}_{i\mu} q_\mu(t)$  in the  $x$ - $y$  plane, with magnitude  $\omega_{i\perp} \ll \omega_0$  and  $|d \ln \omega_{i\perp} / dt| \ll \omega_0$ , as we may safely assume that Eq. (3) is dominated by paths  $Q(t)$  varying slowly on the  $\omega_0^{-1}$  time scale. This permits us to evaluate  $A_i[Q(t)]$  using an adiabatic approximation. We may further take the instantaneous precession axis of the spin as  $\hat{\mathbf{z}}$  for all  $t$  with negligible error (of order  $\omega_{i\perp}/\omega_0$ ). It is far more important to approximate the phase well. The instantaneous energies of the states  $|\pm\rangle_i$  are given by  $\pm(\omega_0 + \omega_{i\perp}^2/2\omega_0)$  to relative or-

der  $\omega_{i\perp}^2/\omega_0^2$ . We thus obtain  $A_i = \cos \Phi_i(t)$  with

$$\Phi_i(t) = \int_0^t dt' \omega_{i\perp}^2(t')/4\omega_0. \quad (6)$$

Equation (6) holds for  $t < O(8\omega_0^3/\langle \dot{\omega}_{i\perp}^2 \rangle)$ , where  $\langle \rangle$  denotes an average value, and the dot denotes  $d/dt$ . (The results obtained below imply that this time scale exceeds  $\tau_d$ .) We have also omitted a negligible Berry phase term [11].

It now pays to rearrange the expression for  $P(t)$ . First, we write  $\cos \Phi_i$  as a sum of  $e^{\pm i\Phi_i}$ , and substitute the resulting expression for  $A[Q(t)]$  in Eq. (3). This yields

$$J(Q_f, Q'_f; Q, Q') = \frac{1}{2^{2N}} \sum_{\{s\}, \{s'\}} K_{\{s\}}(Q_f, Q) K_{\{s'\}}^*(Q'_f, Q'), \quad (7)$$

with

$$K_{\{s\}}(Q_f, Q) = \int_Q^{Q_f} [dQ] \exp\left(iS_0[Q(t)] + i \sum_{i,\mu,\nu} s_i u_{\mu\nu}^i \int_0^t q_\mu(t) q_\nu(t) dt\right). \quad (8)$$

In Eqs. (7) and (8),  $\{s\} = (s_1, s_2, \dots, s_N)$ ,  $\{s'\}$  is similarly given, each  $s_i = \pm 1$  is an Ising-like variable, and  $u_{\mu\nu}^i = \mathbf{c}_{i\mu} \cdot \mathbf{c}_{i\nu}/\omega_0$ . Next we define the following combination of propagators,

$$R_{\{s,s'\}}(Q, Q') = \int dQ_f K_{\{s\}}(Q_f, Q) K_{\{s'\}}^*(Q_f, Q'), \quad (9)$$

in terms of which  $P(t)$  can be written as [see Eqs. (5) and (7)]

$$P(t) = \frac{1}{2^{2N}} \sum_{\{s\}, \{s'\}} \int \int dQ dQ' R_{\{s,s'\}}(Q, Q') \rho(Q, Q'). \quad (10)$$

It is apparent that  $K_{\{s\}}$  is the propagator for a set of coupled harmonic oscillators, described by a Hamiltonian that depends on the Ising configuration  $\{s\}$ :

$$H_{\text{nm}}(\{s\}) = \sum_\mu \frac{p_\mu^2}{2m} + \frac{1}{2} \sum_{\mu,\nu} q_\mu (\Omega^2)_{\mu\nu} q_\nu, \quad (11)$$

$$(\Omega^2)_{\mu\nu} = m\omega_\mu^2 \delta_{\mu\nu} - 2 \sum_i s_i u_{\mu\nu}^i. \quad (12)$$

We can thus write  $R_{\{s,s'\}}$  alternatively as

$$R_{\{s,s'\}}(Q, Q') = \langle Q' | e^{iH_{\text{nm}}(\{s'\})t} e^{-iH_{\text{nm}}(\{s\})t} | Q \rangle. \quad (13)$$

Since Eq. (13) only involves harmonic oscillators, we can evaluate it exactly by reverting to path integrals. The exact answer involves trigonometric functions and determinants of the matrices  $\Omega(\{s\})$  and  $\Omega(\{s'\})$  and is of limited use because of the remaining sum on the  $s$ 's. To make further progress, we employ an approximation in the same spirit as that used to obtain the spin transition amplitude  $A_i(Q[t])$ . That is to say that accuracy in the normal mode frequencies is much more important than in the normal modes themselves. Errors in the former lead to errors in  $K_{\{s\}}$  and  $R_{\{s,s'\}}$  that grow with time, while errors in the latter do not. We therefore treat the second term in Eq. (12) as a perturbation, and use the unperturbed normal modes, but correct the frequencies to first order:  $\omega'_\mu = \omega_\mu - \sum_i s_i u_{\mu\mu}^i / m\omega_\mu$ . [Given the stated assumptions about the relative sizes of the three terms in Eq. (1), the frequency shift can indeed be seen to be small.] With this approximation, the kernel  $R_{\{s,s'\}}$  factorizes into a product  $\prod_\mu R_\mu$  of kernels for each mode (we suppress the Ising variables where no confusion is possible), with

$$R_\mu(q'_\mu, q_\mu) = \langle q'_\mu | e^{iH_\mu(\{s'\})t} e^{-iH_\mu(\{s\})t} | q_\mu \rangle, \quad (14)$$

and  $H_\mu = p^2/2m + m\omega_\mu^2 q^2/2$ . Equation (14) has a simple physical interpretation. Starting from an initial state, the system evolves forward in time for a duration  $t$  as a harmonic oscillator of frequency  $\omega_1$ , say. It then evolves backward in time for duration  $t$  as a harmonic oscillator of slightly different frequency  $\omega_2$ . For our problem, this difference propagator,  $R_\mu$ , can be further simplified because the frequencies  $\omega_1$  and  $\omega_2$  are almost identical [14]. If we think about the corresponding classical problem in phase space, the forward and backward evolutions take place on ellipses of nearly equal eccentricity. To good approximation, we may regard the ellipses as coincident. With suitably scaled  $p$  and  $q$  axes, this common ellipse is a circle, on which the particle sweeps out angles  $\omega_1 t$  and  $-\omega_2 t$  in the forward and backward motions. The net evolution is that of a single harmonic oscillator of frequency  $\delta_\mu = \omega_2 - \omega_1$ , and mass  $m\omega_\mu/\delta_\mu$ , for a time  $t$  [15]. In other words,

$$R_\mu(q'_\mu, q_\mu) \approx \langle q'_\mu | e^{i(p_\mu^2 + m^2 \omega_\mu^2 q_\mu^2) \delta_\mu t / 2m\omega_\mu} | q_\mu \rangle. \quad (15)$$

It is now easy to carry out the coordinate integrals in Eq. (10) for the special case where  $\rho$  is a thermal equilibrium density matrix  $\propto e^{-\beta H_{\text{nm}}}$  with  $\beta = 1/kT$ . Since  $\rho$  and  $R$  both factorize by normal mode, i.e.,  $\rho = \prod_\mu \rho_\mu$ , and  $R = \prod_\mu R_\mu$ , the summand in Eq. (10) also factorizes into  $\prod_\mu \Lambda_\mu(t)$ , where  $\Lambda_\mu = \int \int R_\mu \rho_\mu dq_\mu dq'_\mu$ . By using standard coordinate representations of the harmonic oscillator density matrix and propagator,  $\Lambda_\mu$  is easily evaluated, and the result can be written as (restoring  $\hbar$ )

$$P(t) = 2^{-2N} \sum_{\{s,s'\}} \prod_\mu \Lambda_\mu(t), \quad (16)$$

$$\Lambda_\mu(t) = \frac{\sinh \beta \hbar \omega_\mu / 2}{\sinh(\beta \hbar \omega_\mu - i \delta_\mu t) / 2}. \quad (17)$$

Note that  $\delta_\mu = \sum_i (s_i - s'_i) u_{\mu\mu}^i / m\omega_\mu$  depends on the Ising configuration, and  $u_{\mu\mu}^i$  is given below Eq. (8).

Equations (16) and (17) formally answer the question we set out to investigate, but the sum on the  $s$ 's is nontrivial. Some general properties of the result are worth noting, however. Thus,  $P(t)$  is real, and since  $|\Lambda_\mu(t)| \leq 1$ ,  $P(t) \leq 1$ . [In fact,  $P(t) = 1$  only if  $\sum_i u_{\mu\mu}^i t / \pi \omega_\mu$  is an integer for all  $\mu$  simultaneously.] The expressions simplify greatly at  $T = 0$ . Then,  $\Lambda_\mu(t) = e^{i \delta_\mu t / 2}$ , and

$$P(t) = \prod_i \cos^2(\xi_i^2 t / 2\omega_0) \quad (T = 0), \quad (18)$$

$$\xi_i^2 = \sum_\mu \xi_{i\mu}^2 = \sum_\mu \mathbf{c}_{i\mu} \cdot \mathbf{c}_{i\mu} / m\hbar\omega_\mu. \quad (19)$$

Note that  $\xi_i$  and  $\xi_{i\mu}$  have dimensions of frequency. We can also obtain the decoherence time  $\tau_d$  for all  $T$  by examining the initial drop of  $P(t)$  from unity. Writing  $1 - P(t) \approx (t/\tau_d)^2$ , we obtain

$$\frac{1}{\tau_d^2} = \frac{1}{4\omega_0^2} \sum_i \left[ \left( \sum_\mu \xi_{i\mu}^2 \coth x_\mu \right)^2 + \sum_\mu \xi_{i\mu}^4 \operatorname{cosech}^2 x_\mu \right], \quad (20)$$

where  $x_\mu = \beta \hbar \omega_\mu / 2$ . Note that  $\tau_d$  falls as  $T$  rises, as it should. At  $T = 0$ ,  $\tau_d^{-2} = \sum_i \xi_i^4 / 4\omega_0^2$ .

We still need the couplings  $\mathbf{c}_{i\mu}$ . These depend on the nature of states  $|e\rangle$  and  $|g\rangle$ , so we will find them only for a particularly favorable situation obtained by using  $\text{Ba}^+$  ions, and states with  $\Delta M = \pm 1$  in the  $6s^2 S_{1/2}$  and  $5d^2 D_{5/2}$  (or  $2D_{3/2}$ ) multiplets for  $|g\rangle$  and  $|e\rangle$ , respectively. The  $2D_{5/2} \rightarrow 2S_{1/2}$  decay is an  $E2$  process, with  $\tau_{\text{sp}} \approx 35$  s [16], and  $\omega_0/2\pi = 1.7 \times 10^{14}$  Hz. The interaction Hamiltonian is given by

$$H' = q \sum_{i,j} \sum_{\alpha=x,y} z_{ij}^{-4} u_\alpha^{ij} \hat{Q}_{\alpha z}^i, \quad (21)$$

where  $q$  is the ionic charge,  $z_i$ ,  $\hat{Q}_{\alpha\beta}^i$ , and  $u_\alpha^i$  are the equilibrium position, quadrupole moment tensor, and displacement from equilibrium of the  $i$ th ion;  $z_{ij} = z_i - z_j$ ,  $u_\alpha^{ij} = u_\alpha^i - u_\alpha^j$ . Note that only transverse vibrations appear in Eq. (21) because states  $|e\rangle$  and  $|g\rangle$  are connected by  $|\Delta M| = 1$ ; the same restriction ensures that the equilibrium quadrupole fields do not drive any  $|e\rangle \leftrightarrow |g\rangle$  transitions. Writing the mode index  $\mu = (r, \alpha)$ , with  $r = 1, 2, \dots, N$ , we can write  $u_\alpha^i = \sum_r F_r^i q_{r\alpha}$ , where the  $F_r^i$  are normal mode eigenvectors [17]. We scale these to obey  $\sum_r F_r^i F_r^j = \delta_{ij}$ ,  $\sum_i F_r^i F_s^i = \delta_{rs}$ . With  $F_r^{ij} \equiv F_r^i - F_r^j$ , and  $Q_{\alpha\beta}^i \equiv \langle e | \hat{Q}_{\alpha\beta}^i | g \rangle$ , we obtain  $|\mathbf{c}_{i,r\alpha}| = -q \sum_j F_r^{ij} z_{ij}^{-4} |Q_{\alpha z}^i|$ .

It remains to substitute the above expression for  $\mathbf{c}_{i,r\alpha}$  into Eqs. (19) and (20) to obtain  $\tau_d$ . In general, this is a

straightforward, if lengthy, numerical procedure. Here we will only outline a simplified calculation at  $T = 0$ . The steps are as follows. First, in Eq. (19) we replace  $\omega_\mu$  by  $\omega_{i,N}$ , the frequency of the zigzag transverse mode, for all  $\mu$ . Since  $\omega_{i,N}$  is the smallest normal mode frequency, this replacement yields a lower bound for  $\tau_d$ . It also obviates finding the  $F_r^i$ , as the sum over  $r$  can be done by orthonormality of the  $F_r^i$ . Second, for the states in question  $|Q_{\alpha z}^i|^2 = 18\hbar/k_0^5\tau_{\text{sp}}$ , with  $k_0 = \omega_0/c$ , and  $\alpha = x, y$ . Third, we note that if  $\omega_z$  is the longitudinal CM vibrational frequency,  $d_0 = (q^2/m\omega_z^2)^{1/3}$  is a natural trap length scale. We define the dimensionless sums  $S_n(i) = \sum_j z_{ij}^{-n} d_0^n$ . (The expression for  $\tau_d^{-2}$  contains a factor  $\sum_i [S_4^2(i) + S_8(i)]^2$ .) We estimate  $S_n(i)$  using a continuum approximation for the ion array [18]. In this approximation, the local interionic spacing is  $s(z) = s(0)(1 - z^2/L^2)^{-1}$ , where  $s(0) = 4L/3N$ , and  $2L$  is the total length of the array, with  $L^3 \approx 3N \ln(0.8N)$ . (All lengths are in units of  $d_0$ .) This yields  $S_n(i) \approx 2\zeta(n)/s^n(z_i)$ . The sum over  $i$  can now be estimated by an integral. Combining these results, we obtain a bound for  $\tau_d$  entirely in terms of trap and ion parameters,

$$\frac{1}{\tau_d} < 0.36 \frac{1}{\tau_{\text{sp}}} \frac{N^{35/6}}{[\ln(0.8N)]^{8/3}} \frac{\omega_z^2}{\omega_0 \omega_{i,N} (k_0 d_0)^5}. \quad (22)$$

The last step is to estimate  $\omega_{i,N}$ . By considering the transverse force on the central ion, we get  $\omega_{i,N}^2 \approx \omega_i^2 - c(N)\omega_z^2$ , where  $\omega_i$  is the CM transverse vibrational frequency, and  $c(N) = 9\zeta(3)N^2/16 \ln(0.8N)$ . In fact, requiring  $\omega_{i,N} > 0$  gives the critical  $\omega_i$  ( $\omega_{i,\text{cr}}$ ) needed to avoid the zigzag instability [18]. The numerical value of  $\tau_d$  implied by Eq. (22) is a very sensitive function of  $\omega_z$  ( $\sim \omega_z^{-16/3}$ ). By choosing  $\omega_{i,N} \approx \omega_{i,\text{cr}}/2$ , and  $\omega_z/2\pi$  in the 10–100 kHz range, the ratio  $\tau_d/\tau_{\text{sp}}$  is seen to lie in the  $10^4$ – $10^8$  range for  $N = 1000$ . [The assumptions behind Eqs. (6), (14), and (15) can all be seen to hold.]

We thus see that contrary to what might have been expected, vibrations of the ions are not a significant source of decoherence in the CZ QC for  $N \leq 1000$ , at least at low enough temperatures. Larger  $N$  values pose serious technical challenges in trap design and in keeping  $s(0)$  large enough to be optically resolvable. The conclusions of the present paper, however, can only be encouraging for the prospect of quantum computation.

I am grateful to H.J. Kimble and D. Wineland for useful comments and correspondence. This work is supported by NSF Grant No. DMR-9306947.

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