

# Quantum dynamics of cold trapped ions with application to quantum computation

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**Abstract.** The theory of interactions between lasers and cold trapped ions as it pertains to the design of Cirac–Zoller quantum computers is discussed. The mean positions of the trapped ions, the eigenvalues and eigenmodes of the ions’ oscillations, the magnitude of the Rabi frequencies for both allowed and forbidden internal transitions of the ions, and the validity criterion for the required Hamiltonian are calculated. Energy level data for a variety of ion species are also presented.

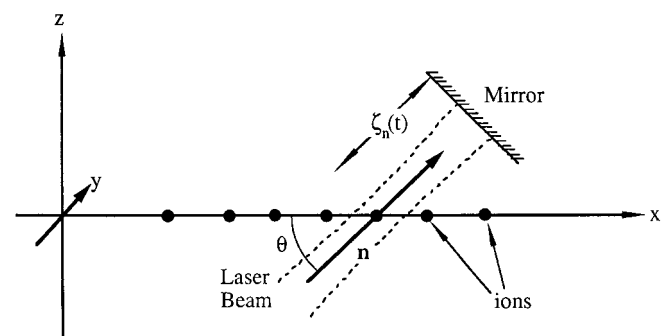
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A quantum computer is a device in which data can be stored in a network of quantum mechanical two-level systems, such as spin-1/2 particles or two-level atoms. The quantum mechanical nature of such systems allows the possibility of a powerful new feature to be incorporated into data processing, namely, the capability of performing logical operations upon quantum mechanical superpositions of numbers. Thus in a conventional digital computer each data register is, throughout any computation, always in a definite state “1” or “0”; however in a quantum computer, if such a device can be realized, each data register (or “qubit”) will be in an undetermined quantum superposition of two states,  $|1\rangle$  and  $|0\rangle$ . Calculations would then be performed by external interactions with the various two-level systems that constitute the device, in such a way that conditional gate operations involving two or more different qubits can be realized. The final result would be obtained by measurement of the quantum mechanical probability amplitudes at the conclusion of the calculation. Much of the recent interest in practical quantum computing has been stimulated by the discovery of a quantum algorithm that allows the determination of the prime factors of large composite numbers efficiently [1] and of coding schemes that, provided operations on the qubits can be performed within a certain threshold degree of accuracy, will allow arbitrarily complicated quantum computations to be performed reliably *regardless of operational error* [2].

So far, the most promising hardware proposed for implementation of such a device seems to be the cold-trapped

ion system devised by Cirac and Zoller [3]. Their design, which is shown schematically in Fig. 1, consists of a string of ions stored in a linear radiofrequency trap and cooled sufficiently so that their motion, which is coupled together due to the Coulomb force between them, is quantum mechanical in nature. Each qubit would be formed by two internal levels of each ion, a laser being used to perform manipulations of the quantum mechanical probability amplitudes of the states, conditional two-qubit logic gates being realized with the aid of the excitation or de-excitation of quanta of the ions’ collective motion. For a more detailed description of the concept of cold-trapped ion quantum computation, the reader is referred to the article by Steane [4].

There are two distinct possibilities for the choice of the internal levels of the ion: first, the two states could be the ground state and a metastable excited state of the ion (or more precisely, sublevels of these states) and second, the two states could be two nearly degenerate sublevels of the ground state. In the first case, a single laser would suffice to perform the required operations; in the second, two lasers would be required to perform Raman transitions between the states, via a third level. Both of these schemes have advantages: the first, which I will refer to as the “single photon” scheme, has the great advantage of conceptual and experimental simplicity; the second, the “Raman scheme”, offers the advantages of a very low



**Fig. 1.** A schematic diagram of ions in a linear trap to illustrate the notation used in this article

rate for spontaneous decay between the two nearly degenerate states and resilience against fluctuations of the phase of the laser. This later scheme was recently used by the group headed by Dr. D.J. Wineland at the National Institute of Science and Technology at Boulder, Colorado to realize a quantum logic gate using a *single* trapped Beryllium ion [5].

In this article, I will discuss the theory of laser interactions with cold trapped ions as it pertains to the design of a Cirac-Zoller quantum computer. I will concentrate on the “single photon scheme” as originally proposed by those authors, although much of the analysis is also relevant to the “Raman scheme”. Fuller accounts of aspects of this are available in the literature: see, for example, [4, 6, 7]; however the derivation of several results are presented here for the first time. I will also present relevant data gleaned from various sources on some species of ion suitable for use in a quantum computer.

## 1 Equilibrium positions of ions in a linear trap

Let us consider a chain of  $N$  ions in a trap. The ions are assumed to be strongly bound in the  $y$  and  $z$  directions but weakly bound in an harmonic potential in the  $x$  direction. The position of the  $m$ th ion, where the ions are numbered from left to right, will be denoted  $x_m(t)$ . The motion of each ion will be influenced by an overall harmonic potential due to the trap electrodes and by the Coulomb force exerted by all of the other ions. We will assume that the binding potential in the  $y$  and  $z$  directions is sufficiently strong that motion along these axes can be neglected. However, motion of the ions transverse to the trap axis can be important in some circumstances: Garg [8] has pointed out that such motion can be a source of decoherence; furthermore if a large number of ions are stored in the trap, the transverse vibrations can become unstable, and the ions will adopt a zigzag configuration [9]. Hence the potential energy of the ion chain is given by the following expression:

$$V = \sum_{m=1}^N \frac{1}{2} M v^2 x_m(t)^2 + \sum_{\substack{n,m=1 \\ m \neq n}}^N \frac{Z^2 e^2}{8\pi\epsilon_0} \frac{1}{|x_n(t) - x_m(t)|}, \quad (1)$$

where  $M$  is the mass of each ion,  $e$  is the electron charge,  $Z$  is the degree of ionization of the ions,  $\epsilon_0$  is the permittivity of free space, and  $v$  is the trap frequency, which characterizes the strength of the trapping potential in the axial direction. Note

that this is an unconventional use of the symbol  $v$ , which often denotes frequency rather than angular frequency; following Cirac and Zoller, I will use  $\omega$  to denote the angular frequencies of the laser or the transitions between internal states of the ions, and  $\nu$  to denote angular frequencies associated with the motion of the ions.

Assume that the ions are sufficiently cold that the position of the  $m$ th ion can be approximated by the formula

$$x_m(t) \approx x_m^{(0)} + q_m(t) \quad (2)$$

where  $x_m^{(0)}$  is the equilibrium position of the ion, and  $q_m(t)$  is a small displacement. The equilibrium positions will be determined by the following equation:

$$\left[ \frac{\partial V}{\partial x_m} \right]_{x_m=x_m^{(0)}} = 0. \quad (3)$$

If we define the length scale  $\ell$  by the formula

$$\ell^3 = \frac{Z^2 e^2}{4\pi\epsilon_0 M v^2} \quad (4)$$

and the dimensionless equilibrium position  $u_m = x_m^{(0)}/\ell$ , then (3) may be rewritten as the following set of  $N$  coupled algebraic equations for the values of  $u_m$ :

$$u_m - \sum_{n=1}^{m-1} \frac{1}{(u_m - u_n)^2} + \sum_{n=m+1}^N \frac{1}{(u_m - u_n)^2} = 0 \quad (m = 1, 2, \dots, N). \quad (5)$$

For  $N = 2$  and  $N = 3$ , these equations may be solved analytically:

$$N = 2: \quad u_1 = -(1/2)^{2/3}, \quad u_2 = (1/2)^{2/3}, \quad (6)$$

$$N = 3: \quad u_1 = -(5/4)^{1/3}, \quad u_2 = 0, \quad u_3 = (5/4)^{1/3}. \quad (7)$$

For larger values of  $N$  it is necessary to solve for the values of  $u_m$  numerically. The numerical values of the solutions to these equations for 2 to 10 ions is given in Table 1. Determining the solutions for larger numbers of ions is a straightforward but time consuming task.

By inspection, the minimum value of the spacing between two adjacent ions occurs at the center of the ion chain. Compiling the numerical data for the minimum value of the separation for different numbers of trapped ions, we find that it

**Table 1.** Scaled equilibrium positions of the trapped ions for different total numbers of ions <sup>a</sup>

N	Scaled equilibrium positions									
2										
3										
4										
5										
6										
7										
8										
9										
10										

<sup>a</sup> This data was obtained by numerical solutions of (5). The length scale is given by (4)

obeys the following relation:

$$u_{\min}(N) \approx \frac{2.018}{N^{0.559}}. \quad (8)$$

This relation is illustrated in Figure 2. Thus the minimum inter-ion spacing for different numbers of ions is given by the following formula:

$$x_{\min}(N) = \left( \frac{Z^2 e^2}{4\pi\epsilon_0 M v^2} \right)^{1/3} \frac{2.018}{N^{0.559}}. \quad (9)$$

This relationship is important in determining the capabilities of cold-trapped ion quantum computers [10].

## 2 Quantum fluctuations of the ions

This section discusses the equations of motion that describe the displacements of the ions from their equilibrium positions. Because of the Coulomb interactions between the ions, the displacements of different ions will be coupled together. The Lagrangian describing the motion is then

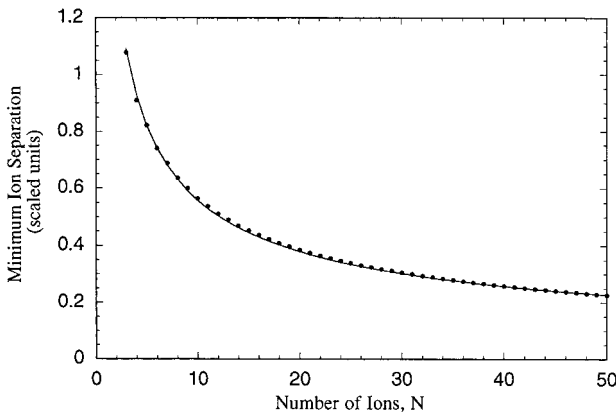
$$L = \frac{M}{2} \sum_{m=1}^N (\dot{q}_m)^2 - \frac{1}{2} \sum_{n,m=1}^N q_n q_m \left[ \frac{\partial^2 V}{\partial x_n \partial x_m} \right]_0, \quad (10)$$

where the subscript 0 denotes that the double partial derivative is evaluated at  $q_n = q_m = 0$ , and we have neglected terms  $O[q_n^3]$ . The partial derivatives may be calculated explicitly to give the following expression:

$$L = \frac{M}{2} \left[ \sum_{m=1}^N (\dot{q}_m)^2 - v^2 \sum_{n,m=1}^N A_{nm} q_n q_m \right], \quad (11)$$

where

$$A_{nm} = \begin{cases} 1 + 2 \sum_{\substack{p=1 \\ p \neq m}}^N \frac{1}{|u_m - u_p|^3} & \text{if } n = m, \\ \frac{-2}{|u_m - u_n|^3} & \text{if } n \neq m. \end{cases} \quad (12)$$



**Fig. 2.** The relationship between the number of trapped ions  $N$  and the minimum separation. The curve is given by (8) while the points come from the numerical solutions of the algebraic equations (5)

Since the matrix  $A_{nm}$  is real, symmetric, and non-negative definite, its eigenvalues must be non-negative. The eigenvectors  $\mathbf{b}_m^{(p)}$  ( $p = 1, 2, \dots, N$ ) are therefore defined by the following formula:

$$\sum_{n=1}^N A_{nm} \mathbf{b}_n^{(p)} = \mu_p \mathbf{b}_m^{(p)} \quad (p = 1, \dots, N), \quad (13)$$

where  $\mu_p \geq 0$ . The eigenvectors are assumed to be numbered in order of increasing eigenvalue and to be properly normalized so that

$$\sum_{p=1}^N \mathbf{b}_n^{(p)} \mathbf{b}_m^{(p)} = \delta_{nm} \quad (14)$$

$$\sum_{n=1}^N \mathbf{b}_n^{(p)} \mathbf{b}_n^{(q)} = \delta_{pq}. \quad (15)$$

The first eigenvector (i.e., the eigenvector with the smallest eigenvalue) can be shown to be

$$\mathbf{b}^{(1)} = \frac{1}{\sqrt{N}} \{1, 1, \dots, 1\}, \quad \mu_1 = 1. \quad (16)$$

The next eigenvector can be shown to be

$$\mathbf{b}^{(2)} = \frac{1}{\left( \sum_{m=1}^N u_m^2 \right)^{1/2}} \{u_1, u_2, \dots, u_N\}, \quad \mu_2 = 3. \quad (17)$$

Higher eigenvectors must, in general, be determined numerically; (15) and (16) imply that

$$\sum_{m=1}^N \mathbf{b}_m^{(p)} = 0 \quad \text{if } p \neq 1. \quad (18)$$

For  $N = 2$  and  $N = 3$ , the eigenvectors and eigenvalues may be determined algebraically:

$$N = 2: \quad \mathbf{b}^{(1)} = \frac{1}{\sqrt{2}}(1, 1), \quad \mu_1 = 1, \\ \mathbf{b}^{(2)} = \frac{1}{\sqrt{2}}(-1, 1), \quad \mu_2 = 3, \quad (19)$$

$$N = 3: \quad \mathbf{b}^{(1)} = \frac{1}{\sqrt{3}}(1, 1, 1), \quad \mu_1 = 1, \\ \mathbf{b}^{(2)} = \frac{1}{\sqrt{2}}(-1, 0, 1), \quad \mu_2 = 3, \\ \mathbf{b}^{(3)} = \frac{1}{\sqrt{6}}(1, -2, 1), \quad \mu_3 = 29/5. \quad (20)$$

For larger values of  $N$ , the eigenvalues and eigenvectors must be determined numerically; their numerical values for 2 to 10 ions are given in Table 2.

The *normal modes* of the ion motion are defined by the formula

$$Q_p(t) = \sum_{m=1}^N \mathbf{b}_m^{(p)} q_m(t). \quad (21)$$

**Table 2.** Numerically determined eigenvalues and eigenvectors of the matrix  $A_{nm}$  defined by (12), for 2 to 10 ions <sup>a</sup>

Eigenvalue		Eigenvector									
N=2	1	( 0.7071,	0.7071)								
	3	(-0.7071,	0.7071)								
N=3	1	( 0.5774,	0.5774,	0.5774)							
	3	(-0.7071,	0,	0.7071)							
	5.8	( 0.4082,	-0.8165,	0.4082)							
N=4	1	( 0.5,	0.5,	0.5,	0.5)						
	3	(-0.6742,	-0.2132,	0.2132,	0.6742)						
	5.81	( 0.5,	-0.5,	-0.5,	0.5)						
	9.308	(-0.2132,	0.6742,	-0.6742,	0.2132)						
N=5	1	( 0.4472,	0.4472,	0.4472,	0.4472,	0.4472)					
	3	(-0.6395,	-0.3017,	0,	0.3017,	0.6395)					
	5.818	( 0.5377,	-0.2805,	-0.5143,	-0.2805,	0.5377)					
	9.332	(-0.3017,	0.6395,	0,	-0.6395,	0.3017)					
	13.47	( 0.1045,	-0.4704,	0.7318,	-0.4704,	0.1045)					
N=6	1	( 0.4082,	0.4082,	0.4082,	0.4082,	0.4082,	0.4082)				
	3	(-0.608,	-0.3433,	-0.1118,	0.1118,	0.3433,	0.608)				
	5.824	(-0.5531,	0.1332,	0.4199,	0.4199,	0.1332,	-0.5531)				
	9.352	( 0.3577,	-0.5431,	-0.2778,	0.2778,	0.5431,	-0.3577)				
	13.51	( 0.1655,	-0.5618,	0.3963,	0.3963,	-0.5618,	0.1655)				
	18.27	(-0.04902,	0.2954,	-0.6406,	0.6406,	-0.2954,	0.04902)				
N=7	1	( 0.378,	0.378,	0.378,	0.378,	0.378,	0.378,	0.378)			
	3	(-0.5801,	-0.3636,	-0.1768,	0,	0.1768,	0.3636,	0.5801)			
	5.829	(-0.5579,	0.031,	0.3213,	0.4111,	0.3213,	0.031,	-0.5579)			
	9.369	(-0.3952,	0.445,	0.3818,	0,	-0.3818,	-0.445,	0.3952)			
	13.55	(-0.213,	0.5714,	-0.1199,	-0.4769,	-0.1199,	0.5714,	-0.213)			
	18.32	( 0.08508,	-0.4121,	0.5683,	0,	-0.5683,	0.4121,	-0.08508)			
	23.66	( 0.02222,	-0.1723,	0.4894,	-0.6787,	0.4894,	-0.1723,	0.02222)			
N=8	1	( 0.3536,	0.3536,	0.3536,	0.3536,	0.3536,	0.3536,	0.3536,	0.3536)		
	3	(-0.5556,	-0.373,	-0.217,	-0.07137,	0.07137,	0.217,	0.373,	0.5556)		
	5.834	(-0.5571,	-0.0425,	0.2362,	0.3634,	0.3634,	0.2362,	-0.0425,	-0.5571)		
	9.383	( 0.4212,	-0.3577,	-0.4093,	-0.1647,	0.1647,	0.4093,	0.3577,	-0.4212)		
	13.58	(-0.2508,	0.5479,	0.0669,	-0.364,	-0.364,	0.0669,	0.5479,	-0.2508)		
	18.37	( 0.1176,	-0.4732,	0.4123,	0.3039,	-0.3039,	-0.4123,	0.4732,	-0.1176)		
	23.73	(-0.04169,	0.2703,	-0.561,	0.3324,	0.3324,	-0.561,	0.2703,	-0.04169)		
	29.63	(-0.009806,	0.09504,	-0.3398,	0.6127,	-0.6127,	0.3398,	-0.09504,	0.009806)		
N=9	1	( 0.3333,	0.3333,	0.3333,	0.3333,	0.3333,	0.3333,	0.3333,	0.3333)		
	3	(-0.5339,	-0.3764,	-0.2429,	-0.1194,	0,	0.1194,	0.2429,	0.3764,	0.5339)	
	5.838	(-0.5532,	-0.09692,	0.1658,	0.3078,	0.3531,	0.3078,	0.1658,	-0.09692,	-0.5532)	
	9.396	(-0.4394,	0.2828,	0.4019,	0.2558,	0,	-0.2558,	-0.4019,	-0.2828,	0.4394)	
	13.6	( 0.2812,	-0.5108,	-0.1873,	0.2228,	0.3881,	0.2228,	-0.1873,	-0.5108,	0.2812)	
	18.41	( 0.1465,	-0.5015,	0.2582,	0.4005,	0,	-0.4005,	-0.2582,	0.5015,	-0.1465)	
	23.79	( 0.06133,	-0.3407,	0.5274,	-0.02271,	-0.4505,	-0.02271,	0.5274,	-0.3407,	0.06133)	
	29.71	(-0.01969,	0.1639,	-0.4614,	0.5098,	0,	-0.5098,	0.4614,	-0.1639,	0.01969)	
	36.16	(-0.004234,	0.05021,	-0.2195,	0.4939,	-0.6408,	0.4939,	-0.2195,	0.05021,	-0.004234)	
N=10	1	( 0.3162,	0.3162,	0.3162,	0.3162,	0.3162,	0.3162,	0.3162,	0.3162,	0.3162)	
	3	(-0.5146,	-0.3764,	-0.26,	-0.153,	-0.05056,	0.05056,	0.153,	0.26,	0.3764,	0.5146)
	5.841	(-0.5476,	-0.1382,	0.1079,	0.2544,	0.3235,	0.3235,	0.2544,	0.1079,	-0.1382,	-0.5476)
	9.408	( 0.4524,	-0.2189,	-0.3786,	-0.3024,	-0.1123,	0.1123,	0.3024,	0.3786,	0.2189,	-0.4524)
	13.63	( 0.3059,	-0.4689,	-0.2629,	0.09726,	0.3287,	0.3287,	0.09726,	-0.2629,	-0.4689,	0.3059)
	18.45	( 0.1721,	-0.5098,	0.1267,	0.3959,	0.194,	-0.194,	-0.3959,	-0.1267,	0.5098,	-0.1721)
	23.85	( 0.08046,	-0.3902,	0.4528,	0.1795,	-0.3225,	-0.3225,	0.1795,	0.4528,	-0.3902,	0.08046)
	29.79	( 0.03062,	-0.2232,	0.505,	-0.3078,	-0.3154,	0.3154,	0.3078,	-0.505,	0.2232,	-0.03062)
	36.26	(-0.009023,	0.09371,	-0.338,	0.5419,	-0.2886,	-0.2886,	0.5419,	-0.338,	0.09371,	-0.009023)
	43.24	( 0.001795,	-0.0256,	0.134,	-0.3656,	0.5897,	-0.5897,	0.3656,	-0.134,	0.0256,	-0.001795)

<sup>a</sup> The eigenvectors are normalized as defined by (15)

The first mode  $Q_1(t)$  corresponds to all of the ions oscillating back and forth as if they were rigidly clamped together; this is referred to as the *center of mass* mode. The second mode  $Q_2(t)$  corresponds to each ion oscillating with an amplitude proportional to its equilibrium distance from the trap center; This is called the *breathing mode*. The Lagrangian for the ion oscillations (11) may be rewritten in terms of these normal modes as follows:

$$L = \frac{M}{2} \sum_{p=1}^N [\dot{Q}_p^2 - \nu_p^2 Q_p^2], \quad (22)$$

where the angular frequency of the  $p$ th mode is defined by

$$\nu_p = \sqrt{\mu_p} \nu. \quad (23)$$

This expression implies that the modes  $Q_p$  are uncoupled. Thus the canonical momentum conjugate to  $Q_p$  is  $P_p = M\dot{Q}_p$  and one can immediately write the Hamiltonian as

$$\hat{H} = \frac{1}{2M} \sum_{p=1}^N P_p^2 + \frac{M}{2} \sum_{p=1}^N \nu_p^2 Q_p^2. \quad (24)$$

The quantum motion of the ions can now be considered by introducing the operators<sup>1</sup>

$$Q_p \rightarrow \hat{Q}_p = i \sqrt{\frac{\hbar}{2M\nu_p}} (\hat{a}_p - \hat{a}_p^\dagger), \quad (25)$$

$$P_p \rightarrow \hat{P}_p = \sqrt{\frac{\hbar M \nu_p}{2}} (\hat{a}_p + \hat{a}_p^\dagger). \quad (26)$$

where  $\hat{Q}_p$  and  $\hat{P}_p$  obey the canonical commutation relation  $[\hat{Q}_p, \hat{P}_p] = i\hbar\delta_{pq}$  and the creation and annihilation operators  $\hat{a}_p^\dagger$  and  $\hat{a}_p$  obey the usual commutation relation  $[\hat{a}_p, \hat{a}_q^\dagger] = \delta_{pq}$ .

Using this notation, the interaction picture operator for the displacement of the  $m$ th ion from its equilibrium position is given by the formula:

$$\begin{aligned} \hat{q}_m(t) &= \sum_{p=1}^N \mathbf{b}_m^{(p)} \hat{Q}_p(t) \\ &= i \sqrt{\frac{\hbar}{2M\nu N}} \sum_{p=1}^N s_m^{(p)} (\hat{a}_p e^{-i\nu_p t} - \hat{a}_p^\dagger e^{-i\nu_p t}), \end{aligned} \quad (27)$$

where the coupling constant is defined by

$$s_m^{(p)} = \frac{\sqrt{N} \mathbf{b}_m^{(p)}}{\mu_p^{1/4}}. \quad (28)$$

For the center of mass mode,

$$s_m^{(1)} = 1 \quad \nu_1 = \nu, \quad (29)$$

<sup>1</sup> There is some arbitrariness in the definition of the operators  $\hat{P}_p$  and  $\hat{Q}_p$ , which is related to the arbitrariness of the phase of the Fock states. I have used the definitions given by Kittel ([11], p. 16), which differs from that given in other texts on quantum mechanics (see, for example, [12] p. 183 or [13] p. 36).

and for the breathing mode

$$s_m^{(2)} = \frac{\sqrt{N}}{\sqrt[4]{3}} \frac{1}{\left(\sum_{m=1}^N u_m^2\right)^{1/2}} u_m \quad \nu_2 = \sqrt{3}\nu. \quad (30)$$

The Lagrangian equation (10) was derived from a Taylor expansion of the potential function about the equilibrium positions of the ions, terms  $O[q_n^3]$  being neglected. The ratio of the strengths of the neglected terms to the strength of the quadratic terms, which are included, is, for low phonon numbers, of the order of  $(\hbar V/8Mc^2 N^3 \alpha^2)^{1/6}$ , where  $\alpha$  is the fine structure constant. Clearly this dimensionless quantity must be small if the approximation we have made is to be valid; for example, if we consider a single Ca II ion in a trap with axial frequency  $\nu = (2\pi) \times 500$  KHz, it has the value  $2.2 \times 10^{-3}$ . The neglected terms will however important because they give a coupling between different phonon modes which may be a source of decoherence.

### 3 Laser-ion interactions

I will now consider the interaction of a laser field with the trapped ions. The theory must take into account both the internal and vibrational degrees of freedom of the ions. I will consider two types of transition between internal ionic levels: the familiar electric-dipole allowed (E1) transitions and dipole forbidden electric quadrupole (E2) transitions. Electric quadrupole transitions have been considered in detail by Freedhoff [14, 15]. The reason for considering forbidden transitions is that they have very long decay lifetimes; spontaneous emission will destroy the coherence of a quantum computer, and therefore is a major limitation on the capabilities of such devices [10, 16]. Magnetic dipole (M1) transitions, which also have long lifetimes, tend only to occur between sub-levels of a configuration and will therefore require, when using the single photon scheme, long wavelength lasers in order to excite them. As it is necessary to resolve individual ions in the trap using the laser, the use of long wavelengths will seriously degrade performance. Transitions between sub-levels of a configuration are however possible using the Raman scheme. More highly forbidden transitions are also a possibility for use in a quantum computer. In particular, there is an octupole allowed (E3) transition of the ion Yb II at 467 nm with a theoretical lifetime of  $1.325 \times 10^8$  sec [17], which has recently been observed at the National Physical Laboratory at Teddington, England [18]. However, such weak transitions can only be excited by either very long laser pulses or by very powerful lasers. Since it is impossible to maintain the phase stability of a laser indefinitely, very long duration pulses (i.e., more than  $\sim 100$  msec) are not practicable. Very high laser power can cause a break-down of the two-level approximation, as highly detuned dipole transitions can become excited. Thus it appears that such *very* long lived states may not in fact give any particular advantages for quantum computing.

The interaction picture Hamiltonians for electric dipole ( $E_1$ ) and electric quadrupole ( $E_2$ ) transitions of the  $m$ th ion,

located at  $x_m$  are

$$\hat{H}_I^{(E1)} = ie \sum_{MN} \omega_{MN} |N\rangle \langle M| \langle N | \hat{r}_i | M \rangle A_i(x_m, t) e^{i\omega_{MN}t}, \quad (31)$$

$$\hat{H}_I^{(E2)} = \frac{ie}{2} \sum_{MN} \omega_{MN} |N\rangle \langle M| \langle N | \hat{r}_i \hat{r}_j | M \rangle \partial_i A_j(x_m, t) e^{i\omega_{MN}t}, \quad (32)$$

where  $A_j(x, t)$  is the  $j$ th component of the vector potential of the laser field,  $\partial_i$  denotes differentiation along the  $i$ th direction and summation over repeated indices ( $i, j = x, y, z$ ) is implied;  $\hat{r}_i$  is the  $i$ th component of the position operator for the valence electron of the ion;  $\{|N\rangle\}$  is the set of all eigenstates of the unperturbed ion and the transition frequency is  $\omega_{MN} = \omega_M - \omega_N$  where the energy of the  $N$ th state is  $\hbar\omega_N$ .

For a laser beam in a standing wave configuration (see Fig. 1), propagating along a direction specified by the unit vector  $\mathbf{n}$ , the vector potential and its derivative are given by the formulas

$$A_i(x_m, t) = -\epsilon_i \frac{E}{i\omega} \sin[k\hat{\zeta}_m(t)] e^{i\omega t} + \text{c.c.}, \quad (33)$$

$$\partial_i A_j(x_m, t) = -n_i \epsilon_j \frac{E}{c} \cos[k\hat{\zeta}_m(t)] e^{i\omega t} + \text{c.c.} \quad (34)$$

In (34), I have approximated the laser beam as a plane wave,  $\epsilon$  being the polarization vector,  $E$  is the amplitude of the electric field,  $\omega$  is the laser frequency and  $k = \omega/c$  is the wavenumber. The operator  $\hat{\zeta}_m(t)$  is the distance between the  $m$ th ion and the plane mirror used to form the standing wave.

If we restrict our consideration to just two states,  $|1\rangle$  and  $|2\rangle$ , and make the rotating wave equation, the interaction Hamiltonians may be rewritten as follows:

$$\hat{H}_I^{(E1)} = \hbar\Omega_0^{(E1)} \sin[k\hat{\zeta}_m(t)] e^{i(t\Delta-\phi)} |1\rangle \langle 2| + \text{h.a.}, \quad (35)$$

$$\hat{H}_I^{(E2)} = i\hbar\Omega_0^{(E2)} \cos[k\hat{\zeta}_m(t)] e^{i(t\Delta-\phi)} |1\rangle \langle 2| + \text{h.a.}, \quad (36)$$

where the detuning is  $\Delta = \omega - \omega_{21}$  and the Rabi frequencies are given by

$$\Omega_0^{(E1)} = \left| \frac{eE}{\hbar} \langle 1 | \hat{r}_i | 2 \rangle \epsilon_i \right|, \quad (37)$$

$$\Omega_0^{(E2)} = \left| \frac{eE\omega_{21}}{2\hbar c} \langle 1 | \hat{r}_i \hat{r}_j | 2 \rangle \epsilon_i n_j \right|. \quad (38)$$

If the standing wave of the laser is so contrived that the equilibrium position of the  $m$ th ion is located at a *node*, i.e., the electric field strength is zero, then

$$\hat{\zeta}_m(t) = l\lambda + \cos\theta \hat{q}_m(t) \quad (39)$$

where  $l$  is some integer,  $\lambda$  is the wavelength, and  $\theta$  is the angle between the laser beam and the trap axis and we have assumed that the fluctuations of the ions transverse to the trap axis are negligible. In this case the two Hamiltonians become

$$\hat{H}_I^{(E1)} = \hbar\Omega_0^{(E1)} k \cos\theta \hat{q}_m(t) e^{i(t\Delta-\phi+l\pi)} |1\rangle \langle 2| + \text{h.a.}, \quad (40)$$

$$\hat{H}_I^{(E2)} = \hbar\Omega_0^{(E2)} e^{i[t\Delta-\phi-(l+1/2)\pi]} |1\rangle \langle 2| + \text{h.a.}, \quad (41)$$

where we have neglected terms involving  $\hat{q}_m(t)^2$ . It is convenient to write the displacement of the ion in terms of the creation and annihilation operators of the phonon modes, viz.,

$$k \cos\theta \hat{q}_m(t) = i \frac{\eta}{\sqrt{N}} \sum_{p=1}^N s_m^{(p)} (\hat{a}_p e^{-iv_p t} - \hat{a}_p^\dagger e^{iv_p t}), \quad (42)$$

where  $\eta = \sqrt{\hbar k^2 \cos^2\theta / 2Mv}$  is called the Lamb–Dicke parameter.

Similarly if the standing wave is arranged so that the ion is at an *antinode*, i.e.,

$$\hat{\zeta}_m(t) = \frac{(2l-1)\lambda}{2} + \cos\theta \hat{q}_m(t), \quad (43)$$

then the Hamiltonians are

$$\hat{H}_I^{(E1)} = \hbar\Omega_0^{(E1)} e^{i(t\Delta-\phi+l\pi)} |1\rangle \langle 2| + \text{h.a.}, \quad (44)$$

$$\hat{H}_I^{(E2)} = \hbar\Omega_0^{(E2)} k \cos\theta \hat{q}_m(t) e^{i[t\Delta-\phi-(l+1/2)\pi]} |1\rangle \langle 2| + \text{h.a.} \quad (45)$$

Thus we have two basic types of Hamiltonian:

$$\hat{H}_V = \hbar\Omega_0 e^{i(t\Delta-\phi_u)} |1\rangle \langle 2| + \text{h.a.}, \quad (46)$$

$$\hat{H}_U = \hbar\Omega_0 k \cos\theta \hat{q}_m(t) e^{i(t\Delta-\phi_u)} |1\rangle \langle 2| + \text{h.a.}, \quad (47)$$

where  $\Omega_0$  stands for either  $\Omega_0^{(E1)}$  or  $\Omega_0^{(E2)}$ .

By changing the node to an antinode, by moving the reflecting mirror, for example, we can switch from one type of Hamiltonian to the other. In the first case, the laser beam will only interact with internal degrees of freedom of the ion, while in the second case the collective motion of the ions will be affected as well.

#### 4 Evaluation of the Rabi frequencies

We can relate the matrix elements appearing in the definitions of the Rabi frequencies to the Einstein  $A$  coefficients for the transitions. In order to do this we will rewrite the matrix elements in terms of the Racah tensors:

$$\langle 1 | \hat{r}_i | 2 \rangle \epsilon_i = \sum_{q=-1}^1 \langle 1 | r C_q^{(1)} | 2 \rangle c_i^{(q)} \epsilon_i, \quad (48)$$

$$\langle 1 | \hat{r}_i \hat{r}_j | 2 \rangle \epsilon_i n_j = \sum_{q=-2}^2 \langle 1 | r^2 C_q^{(2)} | 2 \rangle c_{ij}^{(q)} \epsilon_i n_j, \quad (49)$$

where we have used the fact that  $\epsilon \cdot \mathbf{n} = 0$ . The vectors  $\mathbf{c}^{(q)}$  and the second rank tensors  $c_{ij}^{(q)}$  may be calculated quite easily; explicit expressions are given in the appendix. If we assume  $LS$  coupling, the states  $|1\rangle$  and  $|2\rangle$  are specified by the angular momentum quantum numbers; thus we will use the notation  $|1\rangle = |jm_j\rangle$  and  $|2\rangle = |j'm'_j\rangle$ , where  $j$  is the total angular momentum quantum number and  $m_j$  is the magnetic quantum number of the lower state and  $j'$  is the total angular momentum quantum number and  $m'_j$  the magnetic quantum number of the upper state. Using the Wigner–Eckart theorem ([19],

Section 11.4), the matrix elements may be rewritten as

$$\langle 1|\hat{r}_i|2\rangle\epsilon_i = \langle 1||r\mathbf{C}^{(1)}||2\rangle \sum_{q=-1}^1 \begin{pmatrix} j & 1 & j' \\ -m_j & q & m'_j \end{pmatrix} c_i^{(q)} \epsilon_i, \quad (50)$$

$$\langle 1|\hat{r}_i\hat{r}_j|2\rangle\epsilon_i n_j = \langle 1||r^2\mathbf{C}^{(2)}||2\rangle \sum_{q=-2}^2 \begin{pmatrix} j & 2 & j' \\ -m_j & q & m'_j \end{pmatrix} c_{ij}^{(q)} \epsilon_i n_j, \quad (51)$$

the terms containing six numbers in brackets being Wigner  $3-j$  symbols ([19], Section 5.1), and  $\langle 1||r^q\mathbf{C}^{(q)}||2\rangle$  being the reduced matrix element. The Einstein  $A$  coefficients for the two levels are given by the expressions:

$$\bar{A}_{12}^{(E1)} = \frac{4c\alpha k_{12}^3}{3} \sum_{q=-1}^1 |\langle 1||r\mathbf{C}_q^{(1)}||2\rangle|^2 \quad (52)$$

$$\bar{A}_{12}^{(E2)} = \frac{c\alpha k_{12}^5}{15} \sum_{q=-2}^2 |\langle 1||r^2\mathbf{C}_q^{(2)}||2\rangle|^2. \quad (53)$$

Using the Wigner–Eckart theorem again, these expressions reduce to the following:

$$\bar{A}_{12}^{(E1)} = \frac{4c\alpha k_{12}^3}{3} |\langle 1||r\mathbf{C}^{(1)}||2\rangle|^2 \sum_{q=-1}^1 \begin{pmatrix} j & 1 & j' \\ -m_j & q & m'_j \end{pmatrix}^2 \quad (54)$$

$$\bar{A}_{12}^{(E2)} = \frac{c\alpha k_{12}^5}{15} |\langle 1||r^2\mathbf{C}^{(2)}||2\rangle|^2 \sum_{q=-2}^2 \begin{pmatrix} j & 2 & j' \\ -m_j & q & m'_j \end{pmatrix}^2. \quad (55)$$

These coefficients are the rates for spontaneous decay from the upper level  $|1\rangle$  to the lower level  $|2\rangle$ . A simpler expression for the total rate of spontaneous decay of  $|2\rangle$  to all of the sublevels of the lower state may be found by summing these rates over all values of  $m_j$ :

$$A_{12}^{(E1)} \equiv \sum_{m=-j}^j \bar{A}_{12}^{(E1)} = \frac{4c\alpha k_{12}^3}{3(2j'+1)} |\langle 1||r\mathbf{C}^{(1)}||2\rangle|^2, \quad (56)$$

$$A_{12}^{(E2)} \equiv \sum_{m=-j}^j \bar{A}_{12}^{(E2)} = \frac{c\alpha k_{12}^5}{15(2j'+1)} |\langle 1||r^2\mathbf{C}^{(2)}||2\rangle|^2. \quad (57)$$

These decay rates, which are the same for all of the sublevels of the upper level, are the quantities usually quoted in data tables. Using (37), (38), (50), (51), (56) and (57), we then obtain the following formula for the Rabi frequencies:

$$\Omega_0 = \frac{e|E|}{\hbar\sqrt{c\alpha}} \sqrt{\frac{A_{12}}{k_{12}^3}} \sigma, \quad (58)$$

where

$$\sigma^{(E1)} = \sqrt{\frac{3(2j'+1)}{4}} \left| \sum_{q=-1}^1 \begin{pmatrix} j & 1 & j' \\ -m_j & q & m'_j \end{pmatrix} c_i^{(q)} \epsilon_i^{(q)} \right|, \quad (59)$$

$$\sigma^{(E2)} = \sqrt{\frac{15(2j'+1)}{4}} \left| \sum_{q=-2}^2 \begin{pmatrix} j & 2 & j' \\ -m_j & q & m'_j \end{pmatrix} c_{ij}^{(q)} \epsilon_i^{(q)} n_j \right|. \quad (60)$$

The values of these quantities will be dependent on the choice of states of ions used for the upper and lower levels, and upon the polarization and direction of the laser beam. As a specific example, we will assume that the ions are in a weak magnetic field, which serves to define the  $z$ -direction of quantization. Furthermore, we will assume that the lower level  $|1\rangle$  is the  $m_j = -1/2$  sublevel of a  $^2S_{1/2}$  ground state, the nucleus having spin zero. The upper level for the dipole transition is a sublevel of a  $^2P_{1/2}$  state, while for the quadrupole transition it is a sublevel of a  $^2D_{3/2}$  state:

$$\Omega_0^{(E1)} = \frac{e|E|}{\hbar} \sqrt{\frac{A_{12}^{(E1)}}{4c\alpha k_{12}^3}}, \quad (61)$$

$$\Omega_0^{(E2)} = \frac{e|E|}{\hbar} \sqrt{\frac{A_{12}^{(E2)}}{2c\alpha k_{12}^3}}. \quad (62)$$

## 5 Validity of Cirac and Zoller's Hamiltonian

Equations (42) and (47) give the following expression for the Hamiltonian for the case when the laser standing wave is so configured that it can excite the vibration modes of the ions:

$$\hat{H}_U = \frac{i\eta\hbar\Omega_0}{\sqrt{N}} \sum_{p=1}^N s_m^{(p)} (\hat{a}_p e^{-iv_p t} - \hat{a}_p^\dagger e^{iv_p t}) e^{i(t\Delta - \phi_u)} |1\rangle\langle 2| + \text{h.a.} \quad (63)$$

In their paper [3], Cirac and Zoller assumed that the laser can interact with only the center of mass mode of the ions' fluctuations. This interaction forms a vitally important element of their proposed method for implementing a quantum controlled not logic gate. Thus they used a Hamiltonian of the following form [cf. [3], Eq. (1)]:

$$\hat{H}_U^{(CZ)} = \frac{i\eta\hbar\Omega_0}{\sqrt{N}} (\hat{a}_1 e^{-iv_1 t} - \hat{a}_1^\dagger e^{iv_1 t}) e^{i(t\Delta - \phi_u)} |1\rangle\langle 2| + \text{h.a.} \quad (64)$$

This is an approximate form of (63), in which all of the other "extraneous" phonon modes have been neglected. We will now investigate under what circumstances these modes may be ignored.

We will assume that the wavefunction for a single ion interacting with the laser beam may be written as follows:

$$|\Psi(t)\rangle = \alpha_0(t)|1\rangle|vac\rangle + b_0(t)|2\rangle|vac\rangle + \sum_{p=1}^N \alpha_p(t)|1\rangle|1_p\rangle + \sum_{p=1}^N b_p(t)|2\rangle|1_p\rangle, \quad (65)$$

where  $|1\rangle$  and  $|2\rangle$  are the energy eigenstates of the  $m$ th ion's internal degrees of freedom,  $|1_p\rangle$  is the state of the ions' collective vibration in which the  $p$ th mode has been excited by one quantum, and  $|vac\rangle$  is the vibrational ground state. To avoid ambiguity, the ket for the ion's internal state appears first, the ket for the vibrational state second.

The equation of motion for this wavefunction is

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}_U |\Psi(t)\rangle. \quad (66)$$

By using (63), and assuming that one cannot excite states with two phonons, one obtains the following equations:

$$\dot{\alpha}_0 = \frac{\Omega_0 \eta}{\sqrt{N}} \sum_{p=1}^N s_m^{(p)} \beta_p(t), \quad (67)$$

$$\dot{\beta}_0 = \frac{\Omega_0 \eta}{\sqrt{N}} \sum_{p=1}^N s_m^{(p)} \alpha_p(t), \quad (68)$$

$$\dot{\alpha}_p = -i(v_p - v_1)\alpha_p - \frac{\Omega_0 \eta}{\sqrt{N}} s_m^{(p)} \beta_0(t), \quad (69)$$

$$\dot{\beta}_p = -i(v_p + v_1)\beta_p - \frac{\Omega_0 \eta}{\sqrt{N}} s_m^{(p)} \alpha_0(t). \quad (70)$$

We have assumed that  $\Delta = -v_1$ , so that the laser is tuned to the specific sideband resonance required to perform Cirac and Zoller's universal gate operation ([3], Eq. 3), namely, the two level transition  $|1\rangle_n |1_1\rangle \leftrightarrow |2\rangle_n |vac\rangle$ .

Since  $|\alpha_0(t)|, |\beta_0(t)| \leq 1$ , we can consider the following upper limits on the amplitudes of the states which include excitation of "extraneous" phonon modes (i.e., phonon modes other than the center of mass mode):

$$|\alpha_p(t)| \leq |A_p(t)|, \quad |\beta_p(t)| \leq |B_p(t)|, \quad (71)$$

where

$$\dot{A}_0 + i(v_p - v_1)A_p = -\frac{\Omega_0 \eta}{\sqrt{N}} s_m^{(p)}, \quad (72)$$

$$\dot{B}_0 + i(v_p + v_1)B_p = -\frac{\Omega_0 \eta}{\sqrt{N}} s_m^{(p)}. \quad (73)$$

Solving these equations one finds that

$$|A_p(t)| \leq \frac{2\Omega_0 \eta}{\sqrt{N}(v_p - v_1)} |s_m^{(p)}|, \quad (74)$$

$$|B_p(t)| \leq \frac{2\Omega_0 \eta}{\sqrt{N}(v_p + v_1)} |s_m^{(p)}|. \quad (75)$$

Thus the total probability that "extraneous" modes are excited has the following upper limit:

$$P_{\text{ext}} = \sum_{p=2}^N |\alpha_p(t)|^2 + |\beta_p(t)|^2 \leq 2 \left( \frac{2\Omega_0 \eta}{\sqrt{N}v} \right)^2 \left[ \sum_{p=2}^N \frac{\mu_p + 1}{(\mu_p - 1)^2} (s_m^{(p)})^2 \right], \quad (76)$$

where we have used the definition of the mode frequencies (23) and the fact that the eigenvalue for the center of mass mode is  $\mu_1 = 1$ . This quantity will be different for each ion in the string; taking its average value, we find

$$\bar{P}_{\text{ext}} \equiv \frac{1}{N} \sum_{m=1}^N P_{\text{ext}} \leq 2 \left( \frac{2\Omega_0 \eta}{\sqrt{N}v} \right)^2 \Sigma(N), \quad (77)$$

where we have used the definition of the coupling constants (28) and the orthonormality of the eigenvectors (15).

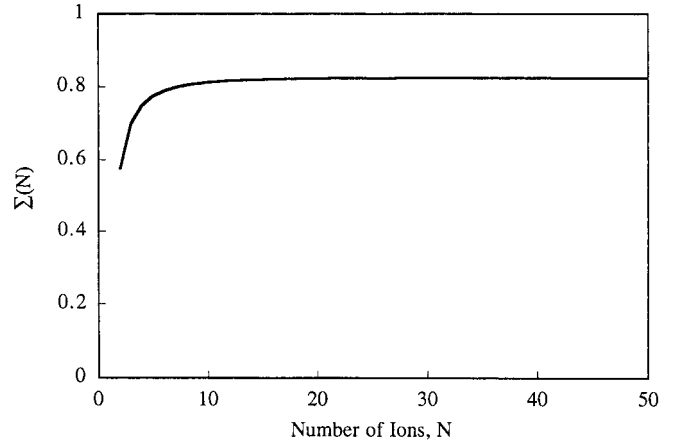


Fig. 3. The function  $\Sigma(N)$  defined by (78)

The function  $\Sigma(N)$  is defined by the formula

$$\Sigma(N) = \sum_{p=2}^N \frac{\mu_p + 1}{(\mu_p - 1)^2 \sqrt{\mu_p}}. \quad (78)$$

This must be evaluated numerically by solving for the eigenvalues of the trap normal modes for different numbers of trapped ions  $N$ . The results are shown in Fig. 3. The function varies slowly with the value of  $N$ , and, for  $N \geq 10$ , we can, to a good approximation, replace it by a constant  $\Sigma(N) \approx 0.82$ . Thus we obtain the following upper limit on the total probability of the "extraneous" phonon modes becoming excited:

$$\bar{P}_{\text{ext}} \leq \left( \frac{2.6\Omega_0 \eta}{\sqrt{N}v} \right)^2. \quad (79)$$

Thus we obtain the following sufficiency condition for the validity of Cirac and Zoller's Hamiltonian (64):

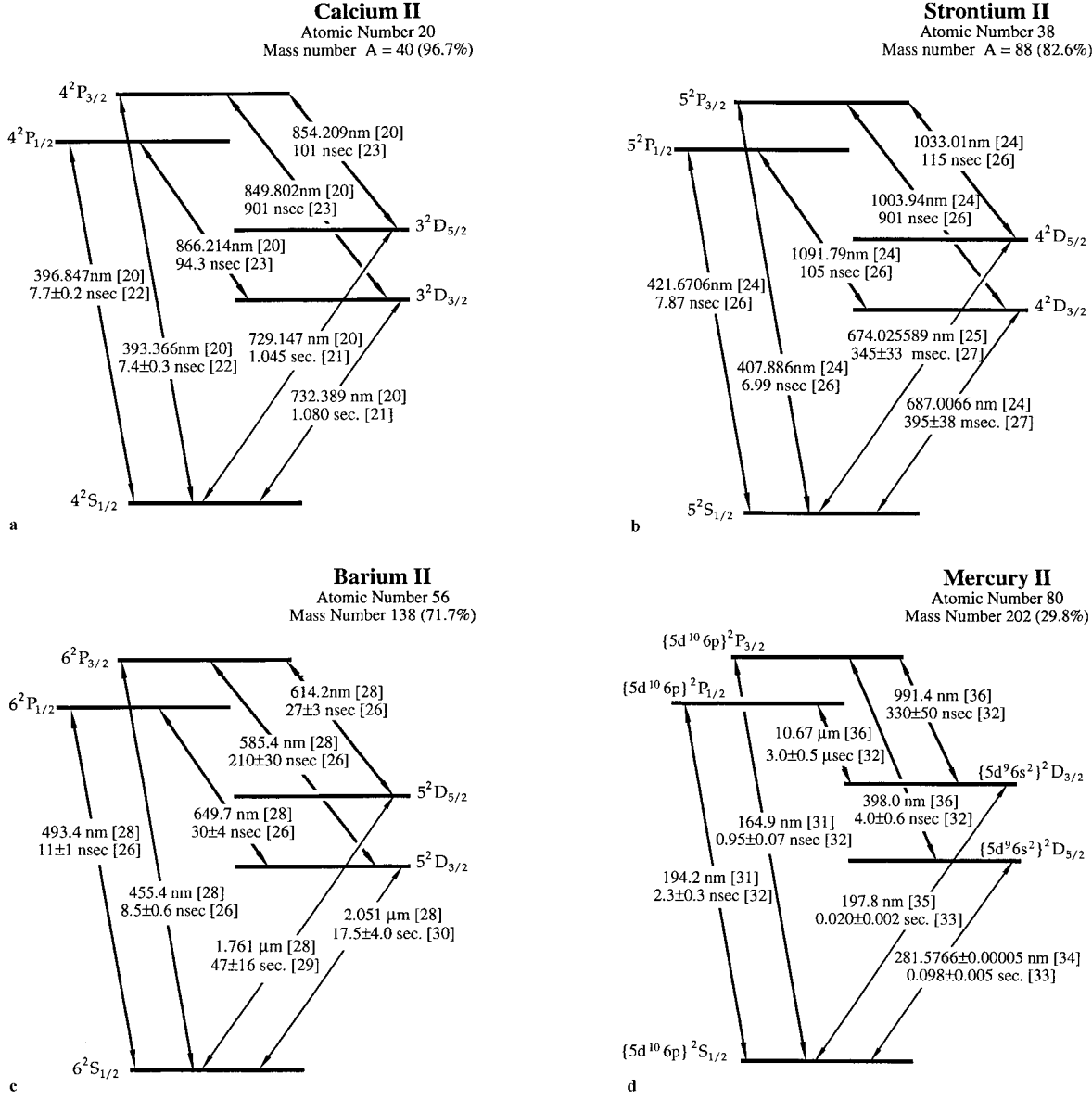
$$\left( \frac{2.6\Omega_0 \eta}{\sqrt{N}v} \right)^2 \ll 1. \quad (80)$$

## 6 Conclusion

In the preceding sections, we have reviewed the theoretical basis for cold-trapped ion quantum computation. How these various laser-ion interaction effects may be combined to perform fundamental quantum logic gates is described in the seminal work of Cirac and Zoller [3]. By using the formulas given here one can determine, for example, the laser field strength required or the separation between ions in the trap. Such things are of great importance in the engineering of practical devices.

Finally there is the question of what type of ion to use. Figure 4 shows the energy levels of four suitable species of ion. These have been chosen based on two criteria: that the lowest excited state has a forbidden transition to the ground state, and their popularity among published ion trapping experiments. It is not intended that this is an exhaustive list of suitable ions, but rather it is to show the properties of typical ions.





**Fig. 4.** Energy level diagrams for four species of ions suitable for quantum computation. Wavelengths and lifetimes are given for the important transitions, the numbers in square brackets being the reference for the data. The lifetime is the reciprocal of the Einstein  $A$  coefficient defined in (56) and (57). The thick lines are dipole allowed ( $E_1$ ) transitions, the thin lines quadrupole allowed ( $E_2$ ) transitions. The atomic number and the mass number of the most abundant isotope (with its relative abundance) are also given. None of these isotopes have a nuclear spin

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## Appendix

The vectors  $\mathbf{c}_i^{(q)}$  are usual normalized spherical basis vectors:

$$\mathbf{c}^{(1)} = -\frac{1}{\sqrt{2}}(1, -i, 0), \quad (\text{A.1})$$

$$\mathbf{c}^{(0)} = (0, 0, 1), \quad (\text{A.2})$$

$$\mathbf{c}^{(-1)} = \frac{1}{\sqrt{2}}(1, i, 0). \quad (\text{A.3})$$

Note that

$$\mathbf{c}^{(q)} = (-1)^q \mathbf{c}^{(-q)*}, \quad (\text{A.4})$$

$$\mathbf{c}^{(q)} \cdot \{\mathbf{c}^{(q')}\}^* = \delta_{q,q'}. \quad (\text{A.5})$$

The second rank tensors  $c_{ij}^{(q)}$  are given by the formula

$$c_{ij}^{(q)} = \sqrt{\frac{10}{3}}(-1)^q \sum_{m_1, m_2=-1}^1 \begin{pmatrix} 1 & 1 & 2 \\ m_1 & m_2 & -q \end{pmatrix} c_i^{(m_1)} c_j^{(m_2)}. \quad (\text{A.6})$$

Explicitly these five tensors are:

$$c_{ij}^{(2)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & -i & 0 \\ -i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{A.7})$$

$$c_{ij}^{(1)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & i \\ -1 & i & 0 \end{pmatrix}, \quad (\text{A.8})$$

$$c_{ij}^{(0)} = \frac{1}{3} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad (\text{A.9})$$

$$c_{ij}^{(-1)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & i \\ 1 & i & 0 \end{pmatrix}, \quad (\text{A.10})$$

$$c_{ij}^{(-2)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & i & 0 \\ i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{A.11})$$

Note that

$$c_{ij}^{(q)} = (-1)^q c_{ij}^{(-q)*}, \quad (\text{A.12})$$

$$\sum_{ij} c_{ij}^{(q)} \{c_{ij}^{(q')}\}^* = \frac{2}{3} \delta_{q,q'}. \quad (\text{A.13})$$

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