Conditional Spin Resonance with Trapped Ions

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Internal states of different ions in an electrodynamic trap are coupled when a static magnetic field is applied – analogous to spin-spin coupling in molecules used for NMR. This spin-spin interaction can be used, for example, to implement quantum logic operations in ion traps using NMR methods. The collection of trapped ions can be viewed as a $N$-qubit molecule with adjustable coupling constants.

I. MOTIVATION

Digital information processing builds upon elementary physical elements (“bits”) that may occupy either one of two possible states labelled 0 and 1, respectively. If a quantum system, for example, an individual atom having discrete energy eigenstates, is chosen as elementary switch (“qu-bit”), then the general state of this system will be a superposition of the two computational basis states, i.e. the states chosen to represent the logic 0 and 1. When applying the superposition principle to a register comprising $N$ qubits, one immediately sees that such a register can exist in a superposition of $2^N$ states thus representing $2^N$ binary encoded numbers simultaneously. Any operation on this register will act on all states at once, effecting parallel processing on an exponentially growing (with $N$) number of states. The outcome of a measurement on this register after such an operation will, of course, yield just one out of $2^N$ possible results with a certain probability.

In order to take advantage of quantum parallelism for efficient computing, a second ingredient is necessary: interference. A useful quantum algorithm has to exploit this parallelism, and, at the same time, make different computational paths interfere such that only the correct result survives after the last computational step [1]. An important example is Shor’s algorithm for the factorization of large numbers [2]. Once created, coherent superpositions have to remain intact while a quantum algorithm is carried out, i.e. qubits must not in an uncontrollable way interact with their environment. This would lead to decoherence, an important issue, not only in the realm of quantum information processing (QIP), but also related to the notion of measurement in quantum mechanics [3].

A quantum computer is ideally suited for the simulation of quantum mechanical systems [4-6], for example, to determine eigenvalues and eigenvectors of many-body systems [6]. Calculating the dynamics of chaotic systems is another useful line of action for a quantum computer, even for one that consists of only a few qubits [6]. Beneficial both for fundamental research and applications is the ability of a quantum computer – comprising a modest number of qubits and working with limited accuracy – to simulate the dynamics of a macroscopic ensemble of classical particles, a task not suitable even for modern supercomputers [6].

In the course of a quantum computation entangled states of qubits are created exhibiting correlations between individual qubits that possess no classical analog. Fundamental questions concerning the role of entanglement, not only in QIP, but also in the framework of general physics [7] add more motivation to exploring the field of QIP. In 1935 Einstein, Podolsky, and Rosen scrutinized quantum mechanical predictions for two entangled particles and found non-local correlations between these particles [11]. This, what Einstein called, ‘spooky action at a distance’ prompted him to call into question quantum theory. During the last decade various experiments succeeded in preparing and analyzing entangled states of different physical systems [12,13], which marked the beginning of controlled manipulation of entanglement of massive particles. On the theoretical side, too, the search for better understanding, quantification, and use of entanglement as a resource for QIP is a very active field [14].

II. TRAPPED IONS AND QIP

QIP is an interdisciplinary field of research, whose results will have significant impact both on basic research and applied sciences. Theory in this field is still well ahead of experimental progress and manageable experimental systems are needed. Essential characteristics of a device designed for quantum computing include [15] the scalability of the

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A. Why is optical radiation used?

Common to all experiments – related either to QIP or other research fields – that require some kind of coupling between internal and external degrees of freedom of atoms is the use of optical radiation for this purpose. The parameter determining the coupling strength between internal and motional dynamics is the so-called Lamb-Dicke parameter

\[ \eta \equiv \sqrt{\frac{(hk)^2}{2m}/h\nu_1} = \Delta z_1 k \]

the square of which gives the ratio between the change in kinetic energy of the atom due to the absorption or emission of a photon and the quantized energy spacing of the harmonic trapping potential characterized by the angular frequency \( \nu_1 \) (\( k \) is the wave vector of the light field, \( m \) the mass of the atom, and \( \Delta z_1 = \sqrt{2m\nu_1} \) signifies the spatial extent of the vibrational ground state wave function of the atom). Only if \( \eta \) is nonvanishing will the absorption or emission of photons be possibly accompanied by a change of the motional state of the atom. This is apparent when the Hamiltonian describing the coupling between an applied electromagnetic field of angular frequency \( \omega \) and a harmonically trapped 2-state atom is considered:

\[ H_I = \frac{1}{2}h\Omega_R(\sigma_+ + \sigma_-) \left[ \exp[i(\eta(a^\dagger + a) - \omega t + \phi')] + \text{h.c.} \right], \]

where \( \Omega_R = \vec{d} \cdot \vec{F}/\hbar \) is the Rabi frequency with \( \vec{d} \cdot \vec{F} \) signifying either magnetic or electric coupling between the atomic dipole and the respective field component. \( \sigma_{+,-} = 1/2 (\sigma_x \pm i\sigma_y) \) are the atomic raising and lowering operators, respectively, \( \Delta z_1(a^\dagger + a) \) is the position operator, and \( \phi' \) is the initial phase of the driving field. Trapping a \(^{171}\text{Yb}^+\) ion, for example, with \( \nu_1 = 2\pi \times 100\text{kHz} \) gives \( \Delta z_1 \approx 17 \text{nm} \) and shows that driving radiation in the optical regime is necessary to couple internal and external dynamics of trapped atoms.

Here, and in the remainder of this article, we consider a Paul trap \([29]\) in a linear configuration where a time-dependent two-dimensional quadrupole field strongly confines the ions in the radial direction yielding an average effective harmonic potential \([30]\). An additional static electric field is chosen such that the ions are harmonically confined also in the axial direction \([31]\). If the confinement of \( N \) ions is much stronger in the radial than in the axial direction, the ions will form a linear chain \([32]\) with typical inter-ion distance \( \delta \) \( \equiv \left( e^2/4\pi\epsilon_0 n_0 \mu^2 \right)^{1/3} \) \([33]\). The distance between neighboring ions \( \delta \) is determined by mutual Coulomb repulsion of the ions and trap frequency \( \nu_1 \) in the axial direction. Manipulation of individual ions is achieved by focusing laser light to a spot size smaller than \( \delta \). Typically, \( \delta \) is of the order of a few \( \mu \text{m} \); for example, \( \delta \approx 7 \mu\text{m} \) for \( N = 10^{10} \) \(^{171}\text{Yb}^+\) ions with \( \nu_1 = 2\pi \times 100\text{kHz} \). Again, only optical radiation is useful for this purpose.
B. Spin resonance

Many phenomena that were only recently studied in the optical domain form the basis for techniques belonging to the standard repertoire of coherent manipulation of nuclear and electronic magnetic moments associated with their spins. One reason for the tremendous and fast success of nuclear magnetic resonance (NMR) experiments in the field of QIP is the high level of sophistication that experimental techniques in this field have reached over decades. This is an impressive example for a successful technology whose basis was developed by physicists \[34\] and that has overcome the boundaries between disciplines of science. For many years researchers, for example, in chemistry and in the life sciences have routinely used commercial NMR equipment. The technological basis for NMR – apart from the preparation of the samples to be investigated – is the generation and coherent manipulation of electromagnetic radiation in the radiofrequency (rf) and microwave (mw) regime. This treasure of knowledge and technology could immediately be exploited, again for fundamental research, in the emerging field of QIP, where even complete algorithms based on quantum logic have been demonstrated \[35,36\].

There are also drawbacks associated with NMR quantum computing, for example, considerable effort has to be devoted to the preparation of pseudo-pure states of a macroscopic ensemble of spins with initial thermal population distribution. This preparation leads to an exponentially growing cost (with the number \( N \) of qubits) either in signal strength or the number of experiments involved \[37\], since the fraction of spins in their ground state is proportional to \( N/2^N \). Extending NMR quantum computing to larger numbers of qubits than in present experiments will also require molecules with more nuclear spins distinct in their resonance frequencies and, at the same time, with appreciable coupling constants.

Trapped ions, on the other hand, provide individual qubits – for example hyperfine states – well isolated from their environment. However, the application of mw radiation for quantum logic operations with a string of ions is not possible, since i) this long wavelength radiation does not couple internal and external degrees of freedom of the ions, and ii) focusing down to the required small spot sizes for access to individual qubits is not possible. It would be desirable to combine the advantages of trapped ions and NMR techniques in future experiments.

III. A MODIFIED ION TRAP

An axial magnetic field gradient applied to an electrodynamic trap indeed has the desired effect of coupling internal state dynamics and motion of the ions when mw driving radiation is applied \[38\]. In addition, the field gradient serves to separate qubit resonances of individual ions making them distinguishable in frequency space. Thus microwave radiation can be used to coherently manipulate hyperfine states of individual ions and condition their internal dynamics on the states of other qubits. The treatment put forward in \[38\] is generalized in what follows and it is shown that mutual spin–spin coupling between qubits arises in such a modified ion trap analogous to the coupling Hamiltonian in molecules used for NMR. The size of this NMR-type coupling is proportional to the square of the ratio between magnetic field gradient \( \partial_z B \) and \( \nu_1 \).

The non-relativistic Hamiltonian describing the internal dynamics of a diatomic molecule may be written as \[39\]

\[
H_M = T_N + T_{el} + V(\vec{r}, R)
\]  

(3)

where \( T_N \) and \( T_{el} \) represent the kinetic energy operator of nuclear and electronic motion, respectively. All electrostatic potential energy terms are contained in \( V(\vec{r}, R) \), with \( \vec{r} \) denoting the collection of electronic coordinates and \( R \) the internuclear distance. Neglecting initially the nuclear kinetic energy yields the Schrödinger equation for the electronic wave functions

\[
(T_{el} + V(\vec{r}, R))\Phi_{el}(\vec{r}, R) \equiv H_{el}(R)\Phi_{el}(\vec{r}, R) = E_{el,a}(R)\Phi_{el}(\vec{r}, R).
\]

(4)

These Born-Oppenheimer (BO) wave functions depend on \( R \) as a parameter. With \( \langle \Phi_{el} | T_N | \Phi_{el} \rangle \chi \approx T_N \langle \Phi_{el} | \Phi_{el} \rangle \chi = T_N\chi \) the Schrödinger equation for the nuclear motional wave functions \( \chi \)

\[
(T_N + E_{el,a})\chi = E\chi
\]  

(5)

determines the dynamics of the nuclei on the BO potential energy curves \( E_{el,a} \).

We now turn to the description of a linear chain of \( N \) harmonically trapped, singly ionized two-level ions in an analogous way. The electronic part of the total Hamiltonian can be solved independently for each ion, since the distance \( \delta \) between different ions is much larger than the extent of individual spatial wave functions. Two Zeeman states, \( |E_{0n}\rangle \) and \( |E_{1n}\rangle \), of each ion serve as one qubit \( n = 1, \ldots, N \). The overall electronic state of the ions obeys \( H_{el}\Phi_{el}(\vec{z}) = E_{el,a}(\vec{z})\Phi_{el}(\vec{z}) \) with
The potential energy relevant for the motion of the ions is obtained from the Pauli matrix. The qubit transition frequency $\omega$ of ions shifts the qubit states $|\Phi_a\rangle$ as long as $\varepsilon$ is much smaller than unity, the eigenfrequencies of the oscillator modes only negligibly depend on $z$. Therefore, only $T_A$ and $V_A$ have to be considered in this case. Expanding $V_A$ around the equilibrium positions $z_{0,n}$ of the ions in terms of $q_n \equiv z_n - z_{0,n}$ up to second order yields the dynamical matrix $\hat{A}$ with $A_{ln} \equiv \partial z_n \partial z_l V_A$ and the Hamiltonian of a harmonic oscillator is obtained

$$T_A + V_A = \frac{1}{2m} \sum_{n=1}^{N} p_{z,n}^2 + \frac{m}{2} \sum_{n=1}^{N} \nu_n^2 Q_n$$  \hspace{1cm} (8)$$

with $N$ uncoupled vibrational modes $\{0\}$. The normal coordinates $\tilde{Q}$ and local coordinates $q$ are connected via $q = \hat{S} \tilde{Q}$ where $\hat{S}$ is the unitary transformation matrix that diagonalizes $\hat{A}$. Further, $P_{Q,n} = m Q_n$.

Taking into consideration the field gradient, a new term in the potential energy arises for ion $j$:

$$\langle \Phi_a | H_{el,j}(\hat{z}) | \Phi_a \rangle = E_{ej}(z_{0,j}) + \frac{\hbar}{2} \frac{\partial \omega_j}{\partial z_j} |_{z_{0,j}} q_j (-1)^{c+1}.$$  \hspace{1cm} (9)$$

An order of magnitude estimate of the size of the additional potential energy term $V_B$ experienced by ion $j$, is obtained upon substitution of $q_j \approx \Delta z_j$ into (9). The new term, $V_B$ has to be compared to $\hbar \nu_1$, the ground state energy of the unperturbed lowest oscillator mode:

$$\varepsilon = \frac{|V_B|}{\hbar \nu_1} = \frac{|\partial \omega_j| \Delta z_j}{\nu_1}.$$  \hspace{1cm} (10)$$

As long as $\varepsilon$ is much smaller than unity, the eigenfrequencies of the oscillator modes only negligibly depend on the additional potential term introduced by the Zeeman shift of the ionic qubit states. Therefore, the part of the Hamiltonian that describes the motional state of the ion string is well approximated by the unperturbed harmonic oscillator, and the complete Hamiltonian reads

$$H = \frac{\hbar}{2} \sum_{n=1}^{N} \omega_n(z_{0,n}) \sigma_{z,n} + \frac{1}{2m} \sum_{n=1}^{N} P_{z,n}^2 + \frac{m}{2} \sum_{n=1}^{N} \nu_n^2 Q_n^2$$

$$+ \frac{\hbar}{2} \sum_{n=1}^{N} \left[ \frac{\partial \omega_n}{\partial z_n} |_{z_{0,n}} \sigma_{z,n} \sum_{l=1}^{N} S_{ln} Q_l \right]$$

$$= \frac{\hbar}{2} \sum_{n=1}^{N} \omega_n(z_{0,n}) \sigma_{z,n} + \frac{1}{2m} \sum_{n=1}^{N} P_{z,n}^2$$

$$+ \frac{m}{2} \sum_{l=1}^{N} \nu_l^2 \left[ Q_l + \frac{\hbar}{2m \nu_l^2} \sum_{n} \frac{\partial \omega_n}{\partial z_n} |_{z_{0,n}} \sigma_{z,n} S_{ln} \right]^2$$

$$- \frac{\hbar}{4m} \sum_{l=1}^{N} \frac{1}{\nu_l^2} \left[ \sum_{n} \frac{\partial \omega_n}{\partial z_n} |_{z_{0,n}} \sigma_{z,n} S_{ln} \right]^2$$  \hspace{1cm} (11)$$
with the electronic energy expanded up to first order in \( q_n \). The unitary transformation \( \tilde{H} = U^\dagger H U \) with

\[
U = \exp \left[ -i \sum_l \left( \frac{1}{2 m \nu_l^2} \sum_n \left. \frac{\partial \omega_n}{\partial z_n} \right|_{z_0,n} \sigma_{z,n} \right) P_{Q,l} \right]
\]

(12)
yields

\[
\tilde{H} = \frac{\hbar}{2} \sum_{n=1}^N \omega_n(z_{0,n})\sigma_{z,n} + \sum_{n=1}^N \frac{P_{Q,n}^2}{2m} + \frac{m}{2} \nu_n^2 \sigma_{Q,n}^2 - H_{SS}.
\]

(13)

Expressing the harmonic oscillator in 13 in terms of creation and annihilation operators \( a_n^\dagger \) and \( a_n \), respectively, using the definitions

\[
\epsilon_{nl} \equiv S_{nl} \frac{\partial \omega_l}{\nu_n} \Delta z_n, \quad \text{and} \quad J_{nl} \equiv \sum_{j=1}^N \nu_j \epsilon_{jn} \epsilon_{jl},
\]

(14, 15)

and after dropping constant terms, \( \tilde{H} \) reads

\[
\tilde{H} = \frac{\hbar}{2} \sum_{n=1}^N \omega_n(z_{0,n})\sigma_{z,n} + \sum_{n=1}^N \hbar \nu_n(a_n^\dagger a_n) - \frac{\hbar}{2} \sum_{n<l}^N J_{nl} \sigma_{z,n} \sigma_{z,l}.
\]

(16)

\( \tilde{H} \) describes a linear string of ions with each ion representing an individually accessible qubit with characteristic resonance frequency. The last term in this Hamiltonian expresses a pairwise coupling between qubits, analogous to the well-known spin-spin coupling in molecules used for NMR experiments. The collection of trapped ions can be viewed as an \( N \)-qubit molecule with adjustable coupling constants (compare section III B).

A. Adding a driving field

The additional term in the Hamiltonian governing the dynamics of qubit \( j \) when irradiated with electromagnetic radiation at frequency \( \omega \) close to its resonance is given by

\[
H_M = \frac{\hbar}{2} \Omega_R (\sigma_j^+ + \sigma_j^-) \left[ \exp[i(kz_j - \omega t + \phi')] + \exp[-i(kz_j - \omega t + \phi')] \right] = \frac{\hbar}{2} \Omega_R (\sigma_j^+ + \sigma_j^-) \left[ \exp \left[ \sum_n i S_{nj} \theta_n(a_n^\dagger + a_n) - i \omega t + \phi \right] + \text{h.c.} \right].
\]

(17)

First performing the unitary transformation \( \tilde{H}_M = U^\dagger H_M U \) where it is convenient to express \( U \) given in 12 as

\[
U = \exp \left[ \frac{i}{2} \sum_{n=1}^N \sum_{l=1}^N \epsilon_{nl} (a_n^\dagger - a_n) \sigma_{z,l} \right],
\]

(18)

then transforming \( \tilde{H}_M \) into the interaction picture defined by \( \tilde{H}_M^I = \exp(\frac{i}{\hbar} \tilde{H}_M) \tilde{H}_M \exp(-\frac{i}{\hbar} \tilde{H}_M) \), and finally omitting terms with time dependent factors that contain the sum of \( \omega \) and \( \omega_j \) (rotating wave approximation) gives

\[
\tilde{H}_M^I = \frac{\hbar}{2} \Omega_R \left[ \exp \left[ i \left( \omega_j - \omega - \frac{1}{2} \sum_n \nu_n \epsilon_{nj} \right) t + i \phi \right] \sigma_j^+ \right. \left. \exp \left[ i \left( \sum_n (\eta_n S_{nj} + i \epsilon_{nj}) a_n^\dagger(t) + (\eta_n S_{nj} - i \epsilon_{nj}) a_n(t) \right) \right] + \text{h.c.} \right].
\]

(19)
with \( a_n(t) = a_n \exp(-i\omega_n t) \) and \( a_n^\dagger(t) = a_n^\dagger \exp(i\omega_n t) \). If the driving radiation \( \omega \) pertains to the rf or mw regime, then \( \eta_n \) is close to zero and the last term in the exponent in \( |1\rangle \) can be neglected (\( \eta_1 \approx 10^{-6} \) for 10 Yb\(^+\) ions with transition frequency \( \omega_0 = 2\pi \times 12.6 \text{ GHz} \) and \( \nu_1 = 2\pi \times 100 \text{kHz} \)). With the definitions

\[
\eta'_n \exp(i\phi_j) \equiv \eta_n S_{nj} + i\epsilon_{nj}, \\
\phi_j \equiv \frac{\pi}{2} - \tan \frac{\eta_n S_{nj}}{\epsilon_{nj}} \approx \frac{\pi}{2},
\]

and \( \Delta_j \equiv \frac{1}{2} \sum_n \nu_n \epsilon_{nj} \) (20)

the Hamiltonian in \( |1\rangle \) can be rewritten as

\[
\tilde{H}_M = \frac{\hbar}{2} \Omega_R \left[ \exp \left[ i(\omega_j + \Delta_j - \omega)t + i\phi \right] \sigma_j^+ \right. \\
\left. \exp \left[ i\sum_n \eta'_n (a_j^\dagger(t)e^{i\phi_j} + a_n(t)e^{-i\phi_j}) \right] + \text{h.c.} \right] \] (21)

The exact value of \( \nu_n \) depends on the internal state configuration of the ion chain. However, after summing over all vibrational modes \( \Delta_j \) in \( |2\rangle \) is nearly independent of the ions’ internal states and reflects a constant shift in the qubit’s resonance frequency. The Hamiltonian \( |2\rangle \) is formally the same as the one valid for the interaction between trapped ions and optical radiation, except that the parameter combination \( \eta_n S_{nj} \) determining the coupling strength between external and internal dynamics has now been replaced by the effective Lamb-Dicke parameter \( \eta'_n \approx \epsilon_{nj} \). Any operation that requires coupling between motion and internal dynamics and thus usually requires optical radiation can be carried out using radiation in the rf or mw regime. For example, conditional quantum dynamics on a collection of qubits may be implemented according to the schemes proposed in \( |17,41,42\rangle \).

Sideband cooling is achieved when combining excitation on the so-called red sideband resonance of an internal ionic transition with a suitable dissipative process, similar to sideband cooling in the optical regime. Optical sideband cooling has proven efficient for the preparation of trapped ions close to their motional ground state \( |19,21\rangle \).

B. Spin resonance with trapped ions

The additional spin–spin coupling term in \( |6\rangle \) is considered to be a disturbance when schemes for quantum logic are applied – specifically designed for trapped ions – that in one way or the other rely on the existence of motional sidebands accompanying qubit transitions. The error introduced by this term is negligible compared to other technological limitations, and does not impose a new limit on the precision of ion trap quantum logic operations \( |33\rangle \).

Instead of employing usual ion trap schemes, this spin-spin coupling term may be directly used to implement conditional dynamics using NMR methods. To obtain an order of magnitude estimate of the coupling constant \( J \) in \( |13\rangle \) we take \( \partial_z \omega_j = (\mu_B/\hbar)\partial_z B \forall j \). Here, state \( |1\rangle \) experiences a linear Zeeman shift and there is no shift for \( |0\rangle \). This is the case, for example, with the ground state of \(^{171}\text{Yb}\) when \( |0\rangle \) and \( |1\rangle \) are identified with \( |S_{1/2}, F = 0 \rangle \) and \( |S_{1/2}, F = 1, m_F = 1 \rangle \), respectively. With \( S_{j_n} \approx N^{-1/2} \approx S_{j_1} \) we obtain

\[
J \approx \frac{1}{4Nm\hbar} \left( \mu_B B \right)^2 \sum_{j=1}^N \frac{1}{\lambda_j^2} \] (22)

where \( \lambda_j^2 \) denotes the \( j \)-th eigenvalue of the dynamical matrix \( \hat{A} \). For 10 \(^{171}\text{Yb}\) ions, \( \nu_1 = 2\pi \times 100 \text{kHz} \), and \( \partial_z B = 10 \text{T/m}, J/2\pi \approx 40 \text{Hz} \). The magnitude of \( J \) is comparable to values that occur in NMR experiments where it depends on the type of molecule and nuclei used. For example, in \( |33\rangle \) \( J/2\pi = 7.2 \text{Hz} \) with protons is quoted; protons and carbon nuclei coupled by \( \tilde{J}_{HC}/2\pi = 103 \text{Hz} \) and \( \tilde{J}_{CC}/2\pi = 201 \text{Hz} \) are described in \( |33\rangle \); values of \( J/2\pi \) ranging from 0.9Hz to 163Hz with the same nuclei in a different molecule are reported in \( |14\rangle \), and protons, nitrogen, carbon, and fluorine nuclei with \( J/2\pi \) between 2.7Hz and 366Hz are described in \( |45\rangle \). Here, \( J \) can be given a desired value by variation of \( \nu_1 \) that characterizes the trapping potential, and of the field gradient \( \partial_z B \). If a gradient is applied that changes with \( z \), then the coupling constants \( J_{ij} \) can assume different values for different pairs of spins.

The variation of the field gradient along the \( z \)-axis is also useful to simultaneously cool all vibrational modes of the ion string \( |46\rangle \).
IV. CONCLUDING REMARKS

Hitherto it was accepted that electromagnetic radiation does not couple internal and motional degrees of freedom of trapped atoms when long-wavelength radiation is used, since the Lamb-Dicke parameter is negligibly small. Here, physical conditions are described under which this coupling does occur for electrodynamically trapped ions and can be used for QIP and other experiments that require coherent conditional dynamics. It has been shown that individual qubits can be distinguished by frequency using microwave radiation.

To date, experiments using spin resonance on the one hand and trapped ions on the other, undoubtedly have been most successful in the implementation of quantum computing. This proposal combines the respective advantages of these two types of experimental techniques: qubits in ion traps can be individually addressed, they are well isolated from the environment, and their number and mutual coupling is variable over a wide range. On the other hand, microwave and radiofrequency technology for NMR experiments has been developed over decades. Thus a new avenue for QIP research is opened up that may lead to simpler and more precise experimental procedures.

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