Realisation of homogeneous ion chain using surface traps.

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In a Radio-Frequency linear ion trap, 1D ion chains are routinely generated in laboratories around the world. They present a non-homogeneous ion density along the chain. The possibility of generating uniformly distributed ion chain, where the distance between any adjacent ions is a constant, would open up new type of experiments in the context of Quantum Information and in the study of the Homogeneous Kibble-Zureck mechanism.

I. INTRODUCTION

Radio-frequency (RF) ion traps are used in many different contexts including quantum computing [1], cold reactions [2], cooling highly charged ions [3], mass spectrometry [4] and quantum simulations [1].

In the context of quantum computing and simulation, novel scalable ion trap architecture, in particular the surface ion trap approach [5] has gained significant traction in recent years. Unlike a 3D linear ion trap geometry, the surface ion traps are relatively easy to micro-fabricate and hence the electrodes can be designed in an arbitrary shape and size [6,8]. However, implementing a large scale quantum algorithms require more than just a scalable ion trap; it is necessary a develop a scalable computing architecture capable of controlling 100-1000s of qubits. Among such architectures, a quantum charged coupled device (QCCD) [9] has recently being realised in a rudimentary application [5]. This requires the ions to be shuttled around while keeping alive the quantum state. This invariably requires full temporal and spatial control over the ion chain, thus requiring a large number of DC electrodes. Separation of two ions in different trapping regions [10], transport of ions around the corners [6] are some of the examples challenges that needs careful consideration. While this approach may be viable for 100s of qubits, it is often challenged by heating of the motional degree of freedom, an essential for two qubit gate operations. An alternative approach is based on distributed computing architecture, where each computing node either implements a QCCD architecture or uses multiple addressing beams for multiple ions without the need to shuttle the ions around [11]. The nodes are then connected via optical quantum communication channels. Considering the later option, the ions are not only addressed individually but also photons are collected from individual ions to create remote entanglement. Therefore, ion separation is an important parameter to consider in distributed computing scheme.

In case of a 1D chain of ion trapped and laser cooled in a harmonic potential, the ions are distributed non-uniformly. The ion-ion distance increases from the trap centre [12] to the edges. Technically, such a configuration is not convenient to address the ions using multiple laser beams. Furthermore, an uniform chain of trapped and laser cooled ions are test-beds for simulating a variety of quantum many body systems like the homogeneous Kibble-Zureck mechanism [13], adiabatic entanglement generation in a Bose-Hubbard model [14] etc. Adiabatic entanglement generation using the Bose-Hubbard model is easier to implement when the hopping probability is uniform over the ion chain, thus requiring uniform distribution of the ions. On the contrary the homogeneous Kibble-Zureck mechanism demands an uniform density of the ions in the chain as it is a strong assumption in the model.

It was first suggested by Lin et al [15] that the use of a quartic rather than a harmonic potential generates a near uniform ion distribution. More recently, Xie et al [16] developed a feedback method to achieve a high degree of homogeneity on a surface trap experiment. Despite these developments, designing electrodes to generate uniform chain of ion with uniformity below 10% remains a challenge. Often, the electric field generated by a non-regular shaped electrodes do not have an analytical solution, making it harder to calculate the required voltages and frequencies to operate such a surface ion trap. Most often, one relies on specialised software based on the Finite Element Method (FEM) or the Boundary Element Methods (BEM), to solve the Laplace/Poisson equations. An alternative numerical approach assumes that there is no gap between the electrodes ; the gap-less(GL) approximation [17], which reflects the reality in case the electrodes are much longer than the real gaps.

Here, we report an alternative approach for designing multi-electrode surface ion trap in order to achieve an homogeneous ion chain. The homogeneity of the chain is aimed at reducing the qubit addressability error from
individual laser beams and more importantly for experiments where the uniform density of strongly coupled oscillators are required such as in the Kibble-Zurek mechanism. The later puts stringent condition on the required uniformity for which the currently available techniques fail.

The article is organised as follows: starting with a brief introduction to the surface ion trap architecture, the novel algorithm to calculate the voltages needed to generate a desired ion chain distribution is presented; It is then used to explore the possibility to obtain the desired topology in function of several experimental constraints and finally, molecular dynamics simulations are used to verify the degree of homogeneity of the ion-chain for various optimal trap parameters as obtained from the novel algorithm.

II. BASICS OF SURFACE ION TRAPS

A Radio-Frequency (RF) linear Paul trap uses a time dependent harmonic potential in three dimensions to generate a time averaged pseudo-potential to confine charge particles in 3D. The stability of the ion on the trap depends on the charge-to-mass ratio of the particle as well as the voltage and frequency of the applied time dependent field. A surface ion trap generates a similar pseudo-potential by planarizing the 3D electrodes to a plane. In this case, see figure 1, the ions are trapped above the surface at a given height, \(h\), corresponding to the location of the minimum of the pseudo-potential, \(V_{PS}(\vec{r})\) at \(\vec{r}\). The \(V_{PS}(\vec{r})\) is given by:

\[
V_{PS}(\vec{r}) = \frac{Q^2}{4\pi m\Omega^2} |\vec{E}_{RF}(\vec{r})|^2
\]

where \(Q\) and \(m\) are the charge and the mass of the trapped particles, and \(\vec{E}_{RF}(\vec{r})\) is the electric field generated by the RF electrodes at \(\vec{r}\).

The methodology to calculate the electric field due to a planar infinite gap-less electrode has been discussed previously in [17, 18]. Essentially, it consists of performing the following surface integral for each surface:

\[
\Phi(x, y, z) = \int \frac{\phi(x', y')|z|}{2\pi((x - x')^2 + (y - y')^2 + z^2)^{3/2}} dx' dy' d\Omega
\]

with the surface potential \(\phi(x, y) = \Phi(x, y, 0)\) known.

For the particular case of a square surface, equation 2 can be solve analytically [17].

Such analytical results are used to compute important parameters, like the height at which the ions will be trapped, \(h\). The parameter \(h\) plays in fact an important role due to the strong dependency of the heating effects on \(h: \propto h^4\) for the anomalous heating [19] and \(\propto h^2\) for Johnson noise [20].

In the context of the GL approximation and for the case of equal width of the two RF electrodes (which is already assumed in figure 1), the value of \(h\) can be obtained analytically [17]: \(h = \sqrt{ab} + a^2\). Notice that the expression of \(h\) depend only on geometric considerations and not on the applied voltages.

The trap depth can also be obtained analytically for this particular case [17] :

\[
V_{depth} = \frac{Q^2}{\pi^2 m \Omega^2} \left( \frac{b}{(a+b)^2 + (a+b)\sqrt{2ab} + a^2} \right)^2
\]

where \(V_{RF}\) and \(\Omega\) are the voltage amplitude and the frequency of the applied voltage on the RF electrode.

Regarding the axial direction, the potential is defined by the control electrodes. Their total number, \(n\), their width \(c\), and the voltages applied on them, \(V_{cc}\) will essentially determine the potential along the trap axis. In the following, we will present a methodology to obtain the \(V_{cc}\) that will best approximate the desired potential.

III. OPTIMIZATION PROBLEM

The objective is, given a number of ions, a desired ion-ion distance, \(d\) and ion height, \(h\), to find a set of parameters, \(n, c\) and \(V_{cc}\) that best approximated the desired experimental situation: that an equally distributed ion chain represents the equilibrium topology.

We start by defining the position of the ions as a uniform chain at \(y = 0, z = h\) and ion-ion distance of \(d\). By imposing that the total force along all directions are equal to zero, we arrive at the following system of equations:
where \( r_i = (x_i, y_i, z_i) \), \( C_i = \frac{k_c Q}{\sum_j \frac{r_{ij}}{|r_{ij}|}} \), \( k_c \) is the Coulomb’s constant and \( E_{CC,x}^{\kappa}(r_i) \) \( E_{CC,y}^{\kappa}(r_i) \) \( E_{CC,z}^{\kappa}(r_i) \) denotes the electric field generated by the control electrode \( \kappa \) in the \( x \), \( y \), \( z \) direction when 1V is applied to it. Similar for the RF and DC electrodes.

The above equations can be re-written as a linear least-squares problem \( 21 \),

\[
\chi^2 = ||Ax - b||^2 \tag{7}
\]

where \( A \) is the design matrix and \( b \) is the target vector.

In order to find the \( V_i \) values that minimise \( \chi^2 \), we have used the optimization solver found on the Scipy package \( 22 \) which allows us to impose bounds on the solutions. While the unbounded linear least-square problems lead to a unique solution based on matrix inversion, the bounded algorithms are iterative. The Scipy solver implements the Trust-Region Reflective algorithm \( 23 \), which iteratively solves trust-region sub-problems based on the on the different variables and the Bounded-Variable least-squares method \( 24 \) where the variables are categorised in free or active, then the algorithm solves the case with the active variables fixed and the free ones as unbounded, effectively solving successively the unconstrained least-square problem. The presence of bounds is a requirement for the active variables fixed and the free ones as unbounded, then the algorithm solves the case with

\[
\sum_{k=1}^{n} V_k E_{CC,x}^{\kappa}(r_i) = -E_{RF,x}^{\kappa}(r_i) - E_{DC,x}^{\kappa}(r_i) \tag{4}
\]

\[
\sum_{k=1}^{n} V_k E_{CC,y}^{\kappa}(r_i) = C_i - E_{RF,y}^{\kappa}(r_i) - E_{DC,y}^{\kappa}(r_i) \tag{5}
\]

\[
\sum_{k=1}^{n} V_k E_{CC,z}^{\kappa}(r_i) = -E_{RF,z}^{\kappa}(r_i) - E_{DC,z}^{\kappa}(r_i) \tag{6}
\]

In the following, we will assume that only a half of the electrodes are operating independently. The other half is paired up. Following the notation of figure 1 it means that \( V_i = V_{-i} \).

For the particular case of 10 independent control electrodes \( n = 10 \), \( h = 100 \mu m \), \( a = 100 \mu m \), \( N = 64 \), \( d_{on} = 10 \mu m \), \( V_{DC} = 0 \), \( V_{RF} = 200V \), \( \Omega/2\pi = 20MHz \) and \( V_{max}/ \), figure 3 shows the evolution of \( \chi^2 \) with the width of the control electrodes, \( c \) (all taken to be equal, except the last outer ones, which are taken to be \( c' = 4c \)). The results of the two different algorithms are shown. The noise on the final residue is explained by the large values of the condition number of the \( A \) matrix, shown in figure 3. In the following, both algorithms will be used and the one with the lower value of \( \chi^2 \) will be kept.

The dependency of \( \chi^2 \) with the electrode width, \( c \) and the maximum allowed control voltage, \( V_{max} \), is shown in figure 5. The other parameters remain the same. We observe that by increasing the maximum voltage allowed, a region can be found with a significantly lower value of \( \chi^2 \) : from \( \chi^2(V_{max} = 60, c = 45\mu m) = 1.5 \cdot 10^{-6} \) to \( \chi^2(V_{max} = 70, c = 45\mu m) = 6 \cdot 10^{-14} \).

Another variable that influences the uniformity, is the number of control electrodes for a fixed value of \( V_{max} \). For the case of \( V_{max} = 80V \), we obtain figure 4.

Notice that in figure 1 there is a region with few number of control electrodes that leads to a very low value of \( \chi^2 \). However, the voltages provided by the optimization algorithm in such cases leads to axial potential depths (APD) that are also very low. For example, for \( c = 45\mu m \) and \( n = 2 \) and \( n = 4 \), the axial potential depth is \( V_{APD} \approx 3.5meV \), while for \( n = 10 \) we obtain \( V_{APD} \approx 70meV \). A higher value of \( V_{APD} \) can be obtained by allowing a higher value \( V_{max} \) : for \( V_{max} = 100V \), \( c = 74\mu m \) and \( n = 10 \), leads to \( V_{APD} \approx 280meV \).

The results regarding the value of \( \chi^2/N \) for a given set of trap and ion chain parameters provide useful information for the decision making during the design process. However, it does not directly provide information about the degree of homogeneity of the ion chain. Such issue is the topic of the next section.
where $\Gamma$ is the friction coefficient due to laser cooling, $\log \chi$ at a height $d$ of an homogenous ion chain with inter-ion distance equal to $\xi$. The trap frequency used is $\Omega/\pi = 10^5$ kHz, $V_{RF} = 200V$, $V_{DC} = 0V$, the friction term used is $\Gamma = 2.0 \cdot 10^{-9} \text{kg/s}$ and the time-step of the Velocity-Verlet algorithm is $dt = \Omega/100 = 2ns$. The final positions after 1 ms simulation are used to evaluate the final inhomogeneity of the ions corresponding to a particular set of $V_{cc}$. The inhomogeneity is defined as the ratio between the spacing standard deviation and the mean of such spacing [26] : $\xi = \Delta \sigma x/\Delta x$. By using the same parameter space as figure 3, we obtain figure 5, where the colour code represents $\log_{10}(100\xi)$.

On the right side of figure 5, two examples of the ion-ion distances are shown. It is clear that the two extremes ions are responsible for a significant increase on the $\xi$ parameter. If such two ions are excluded on the computation of $\xi$, then the $\xi$ parameter would decrease from $3.2\% \rightarrow 1.5\%$ (1.6\% → 0.9\%) for the $V_{cc} = 10V$ ($V_{cc} = 100V$) case shown.

In fact, the two extreme ions can be removed from the optimization problem, i.e., we find the set of $V_{cc}$ that leads to the more homogeneous ion chain, with the exception of the two extreme ions. If we perform again molecular dynamic simulations with such new sets of $V_{cc}$, it leads to figure 6. The range of parameters where the degree of homogeneity is lower than 2\% has significantly increased. Right : Two examples of final configurations. Big Blue Dots : $V_{cc} = 10V$ and $c = 89\mu m$ leading to $\xi = 3.2\%$. Small Orange Dots : $V_{cc} = 100V$ and $c = 80\mu m$ leading to $\xi = 1.6\%$.

IV. MOLECULAR DYNAMIC SIMULATIONS

In the following we will use the values of $V_{cc}$ obtained using the methodology presented above to perform realistic molecular dynamic simulations of the trapped ions. The equations of motion to be solved for each ion $i$, are given by :

$$m\ddot{x}_i = \frac{Q^2}{2} \sum_{j=1,j\neq i}^{N} \frac{x_i - x_j}{|r_i - r_j|^3} + QE^x(r_i) - \Gamma \dot{x}_i$$

$$m\ddot{y}_i = \frac{Q^2}{2} \sum_{j=1,j\neq i}^{N} \frac{y_i - y_j}{|r_i - r_j|^3} + QE^y(r_i) - \Gamma \dot{y}_i$$

$$m\ddot{z}_i = \frac{Q^2}{2} \sum_{j=1,j\neq i}^{N} \frac{z_i - z_j}{|r_i - r_j|^3} + QE^z(r_i) - \Gamma \dot{z}_i$$

(8)

where $\Gamma$ is the friction coefficient due to laser cooling, $r = (x, y, z)$ and the electric field of trap is given by :

$$E^j(r_i) = V_{RF} \cos(\Omega t)E_{k}^{RF,j}(r_i) + V_{cc}E_{k}^{CC,j}(r_i)$$

$$+ \sum_{k=1}^{n} V_{k}E_{k}^{CC,j}(r_i)$$

(9)

where $j$ denotes the orthogonal spatial components $(x, y, z)$. The C code which implements the GL approximation analytical solutions is a modification of a code reported in [25].

The ions are initialised at the desired position, i.e., as an homogenous ion chain with inter-ion distance equal $d$ at a height $h$. The trap frequency used is $\Omega/2\pi = 20MHz$, $V_{RF} = 200V$, $V_{DC} = 0V$, the friction term used is $\Gamma = 2.0 \cdot 10^{-9} \text{kg/s}$ and the time-step of the Velocity-Verlet algorithm is $dt = \Omega/100 = 2ns$. The final

\[\text{Figure 4. Evolution of } \chi^2 \text{ with the number of control electrodes } n, \text{ and their width, } c. \text{ The color axis correspond to } \log \chi^2.\]

\[\text{Figure 5. Left : Dependency of inhomogeneity at the end of MD given by } \xi, \text{ see text for details, versus the maximum voltage allowed, } V_{max}, \text{ and the width of the control electrodes, } c. \text{ The color code indicates } \log 100\xi. \text{ The Black contour represents } \xi = 2\%, \text{ while the Red contour represents the } \xi = 1.75\%. \text{ Right : Two examples of final configurations. Big Blue Dots : } V_{max} = 10V \text{ and } c = 89\mu m \text{ leading to } \xi = 3.2\%. \text{ Small Orange Dots : } V_{max} = 100V \text{ and } c = 80\mu m \text{ leading to } \xi = 1.6\%.\]
V. FROM HARMONIC TRAP TO HOMOGENEOUS ION CHAIN

The set of voltages leading to an homogeneous ion chain are not necessarily the more appropriate choice to trap and cool the ion chain down to ground state. For this reason, we perform molecular dynamic simulations where the ions are initialised in the well known and studied \[27\] harmonic potential, followed by a transition to the values corresponding to the homogeneous ion chain.

The half-length of an ion chain in an harmonic potential of secular frequency, \(\omega\), can be estimated to be \[28\] :

\[
L^3 = \frac{3NQ^2k_C}{m\omega^2}(\ln N + \ln +\gamma_e - 7/2)
\] (10)

We have use an approach similar as above to find the needed voltages to apply in order to obtain an harmonic potential with \(\omega/2\pi = 212kHz\), which should lead to a total ion chain length similar for both the harmonic potential and the homogeneous potential case.

After initializing the ions in the harmonic potential, the simulation waits for 50\(\mu s\) before the transition starts to the new set of voltage values. A transition time of \(t_g = 50\mu s\) has been used. After the transition has finished, the simulation continues during 50\(\mu s\) more. In order to change smoothly the voltages from the harmonic to the homogenous case, we have used an hyperbolic tangent transition, given by \[29,31\] :

\[
V(t) = V_1 + \frac{V_2 - V_1}{2} \left(\frac{\tanh(n_h(2t/t_g - 1))}{\tanh(n_h)} + 1\right)
\] (11)

where \(V_1\) correspond to the set of voltages needed for the harmonic case, \(V_2\) correspond to the set of voltages needed for the homogeneous case and \(n_h\) parameter is used to go from a linear evolution \((n_h = 1)\) to a step function \((n_h \to \infty)\). The evolution of the axial position of the ions is shown in figure 4 where \(n_h = 4\) has been used. It illustrates that the approach proposed should be feasible and applicable to existing surface traps.

VI. CONCLUSION

In summary, we have developed a novel algorithm capable to obtain the control electrodes voltages of a surface ion trap needed to generate, with high fidelity, an uniform ion distribution and an harmonic ion distribution. The approach followed is general and therefore, it should be applicable to a large range of desired ion distributions. The approach is based on local minimization of the total force field at each individual ion position. While the present work has used the obtained the needed electric-fields using the GL approximation, the method can be use electric-fields obtained by FEM/BEM methods to more accurately represent the final geometry.

The validity of the different voltages sets obtained by our method have been cross-checked against a robust molecular dynamics simulation. The simulation results show that even for a relatively large ion number, uniformity below 2% is achievable with only 10 pairs of electrodes and limited voltage applied to them. Therefore, it opens up the possibilities to implement an uniform chain of trapped and laser cooled ions for realizing homogeneous KZM, implementing large scale entanglement using the BHM and scaling up the nodes of a distributed quantum computing architecture.
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