

Classical Optimization Techniques for a Trapped Ion Quantum Simulator

Hin Pok Cyrus Fung¹

¹Department of Physics and Astronomy
University of Waterloo

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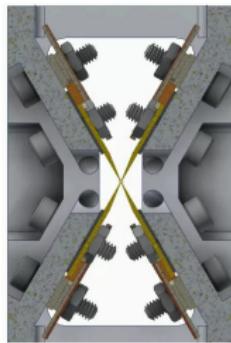
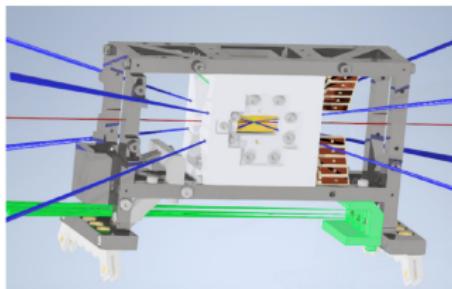
Outline

1 Introduction

Motivation

- Interest in quantum computing (eg Shor's algorithm) and quantum simulation (eg Hubbard model) because of applications
- Ion traps have emerged as a promising platform for both

Example: blade trap



The need for optimization

- Goal: find voltages which generate an electric field that traps the ions in the desired fashion
- 21 parameters: high-dimensional search space
 - Cannot use trial and error
- Use computational optimization

Outline

2 Experimental and Theoretical Techniques

Physics of a blade trap

- U_{blade} : electric potential generated by the blade segments
- Taylor series expansion (using $m = i, j, k$):

$$U_{\text{blade}} = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^4 \beta_{i,j,k} x^i y^j z^k = \sum_m \beta_m x^i y^j z^k$$

- **Important:** identify potential U with its coefficients β_m (vectorized as β), so $U_{\text{blade}} \rightarrow \beta_{\text{blade}}$
- U_{target} : target electric potential ($U_{\text{target}} \rightarrow \beta_{\text{target}}$)

Form of U_{target}

- Ansatz: ion chain; $U = \sum_{i=0}^2 \sum_{j=0}^2 \sum_{k=0}^4 \beta_{i,j,k} x^i y^j z^k$ becomes¹

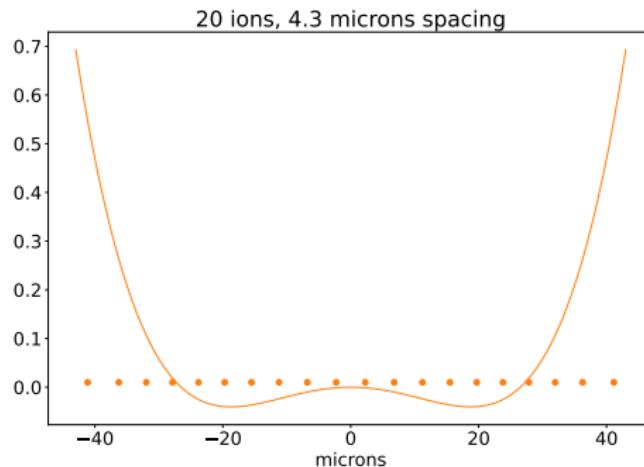
$$U_{\text{target}} = \beta_{2,0,0} x^2 + \beta_{0,2,0} y^2 + \beta_{0,0,2} z^2 + \beta_{0,0,4} z^4$$

Aside: ion equilibrium position

- Minimizes total energy (net force zero)
- $\beta_{0,0,2}$ and $\beta_{0,0,4}$ are optimized such that the ion equilibrium positions are evenly spaced

¹This is why we expand up to x^2, y^2, z^4 .

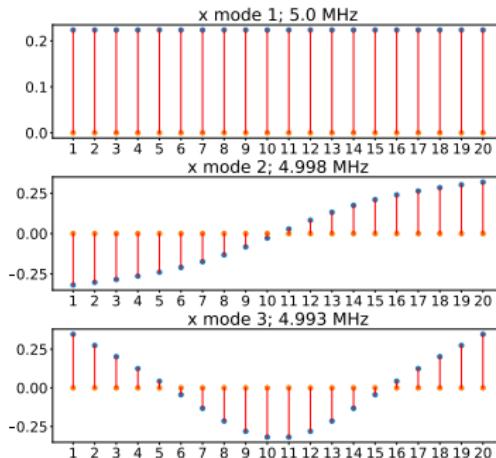
Visualizing $U_{\text{target}} = \beta_{2,0,0}x^2 + \beta_{0,2,0}y^2 + \beta_{0,0,2}z^2 + \beta_{0,0,4}z^4$



Cross section of U_{target} along the z axis (orange curve)
superimposed with the ion equilibrium positions (orange dots)

Center of mass mode

- Vibrations around equilibrium positions: coupled oscillator
- Vibrational (or normal) modes of U_{target} :



- x center of mass (COM) modes are used to couple different qubits; critical to quantum simulation

Linear map from voltages to polynomial coefficients

- Write the 21 voltages as the vector \mathbf{v}
- Write β_m in $U_{\text{blade}} = \sum_m \beta_m x^i y^j z^k$ as the vector $\boldsymbol{\beta}_{\text{blade}}$
- By the superposition principle, $\mathbf{A}\mathbf{v} = \boldsymbol{\beta}_{\text{blade}}$ for some matrix \mathbf{A}

Remark

- \mathbf{A} depends on the layout of the blades^a and is **fixed** as we vary \mathbf{v}

^aColumn vectors of \mathbf{A} are determined by applying 1 Volt to a segment and 0 Volt to others in a simulation.

Solving for \mathbf{v} : voltage optimization

- Given U_{target} , use $\beta_{\text{blade}} := \mathbf{A}\mathbf{v} = \beta_{\text{target}}$ to solve for \mathbf{v}
- But \mathbf{A} is a 45×21 matrix: non-invertible
- Approximate solution $\mathbf{A}\mathbf{v} \approx \beta_{\text{target}}$

Solution: optimization

- Define loss function L which quantifies the “distance”
- Best solution: $\mathbf{v}^* = \operatorname{argmin}_{\mathbf{v}} L(\mathbf{A}\mathbf{v}, \beta_{\text{target}})$
 - $\beta_{\text{blade}} := \mathbf{A}\mathbf{v}^*$ closest to β_{target}

Choice of loss function

Recall: $\mathbf{v}^* = \operatorname{argmin}_{\mathbf{v}} L(\mathbf{A}\mathbf{v}, \boldsymbol{\beta}_{\text{target}})$

- Distance: Euclidean norm $L = \|\mathbf{A}\mathbf{v} - \boldsymbol{\beta}_{\text{target}}\|$
 - Does not work well in practice since it treats all components of $\boldsymbol{\beta}$ equally
- Solution: insert \mathbf{W} weight matrix (fixed during optimization),
 $L = \|\mathbf{W}\mathbf{A}\mathbf{v} - \mathbf{W}\boldsymbol{\beta}_{\text{target}}\|$
 - \mathbf{W} : preprocessing transformation

Outline

3 Results and Discussion

Overview of results section

- Go through a few scenarios to give an idea of experimental considerations

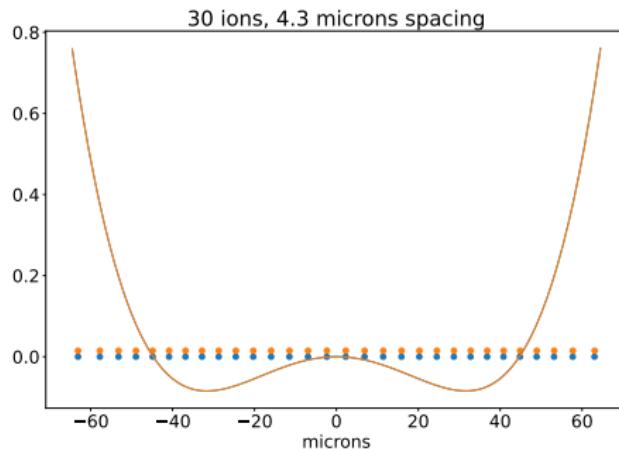
Problem: not enough control

- We want to control 45 parameters β , but we can only adjust 21 parameters \mathbf{v}
- Not enough control \Rightarrow tradeoffs must be made

Criteria

- Equilibrium positions
- COM modes

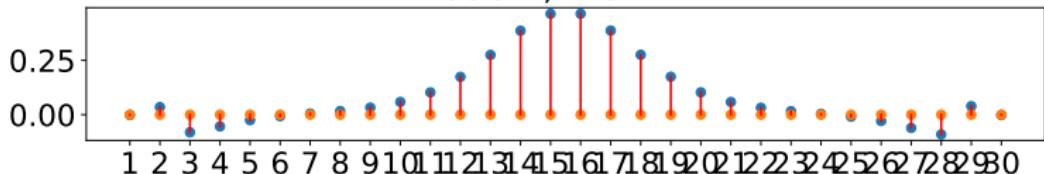
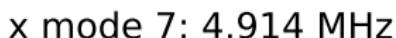
Equilibrium positions of U_{blade} coincide with that of U_{target}



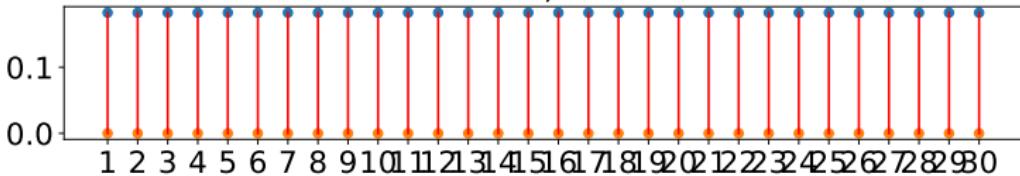
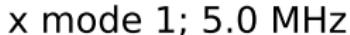
Blue/orange curve: cross section of $U_{\text{blade}}/U_{\text{target}}$ along the z-axis, superimposed with the ion equilibrium positions (blue: U_{blade} , orange: U_{target})

Problem: poor center of mass mode

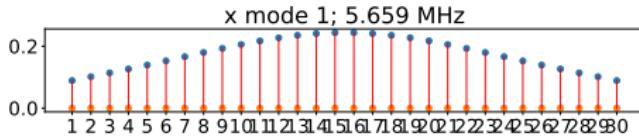
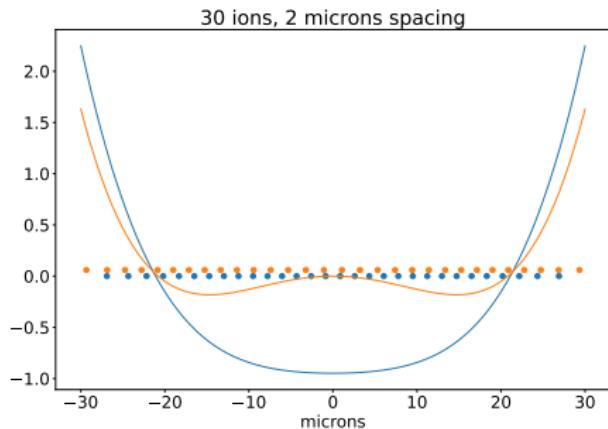
- COM mode of U_{blade} :



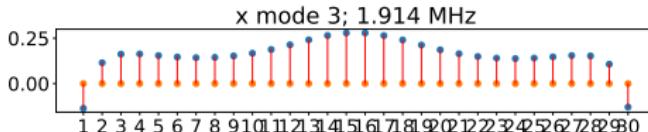
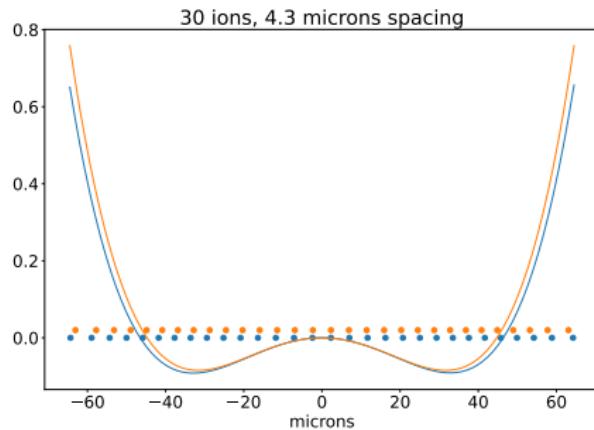
- COM mode of U_{target} :



Solution 1: reduce ion spacing



Solution 2: use weights to suppress x^2z^2 terms



Outline

4 Concluding Remarks

Summary:

- We were able to compute voltages for an ion trap using optimization

Follow-up work

- Problem: matrix \mathbf{A} is computed from simulation, assuming perfect alignment of blades
- During assembly, the blades will not be perfectly aligned, leading to errors
- Solution 1: Measure the actual positions of the blades, rerun the simulation to find \mathbf{A}
- Solution 2: Physical optimization — vary the voltages while keeping track of the ion positions

Thank you!

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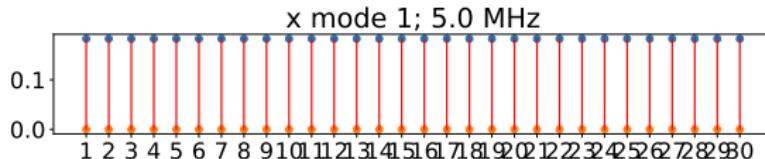
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Outline

5 Appendix

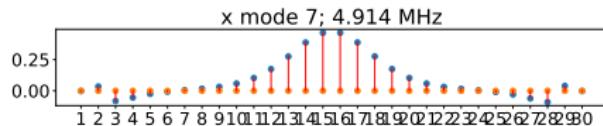
Center of mass mode: details

- We can expand the total energy $U = U_{\text{blade}} + U_{\text{Coulomb}}$ to second order around the equilibrium position
- $[\text{Hess}(\phi)]_{ij} = \frac{\partial^2 U}{\partial q_i \partial q_j}$ is the Hessian of U ; its eigenvectors are the normal modes²
- COM mode refers to the vibrational mode where all the ions move in phase (in the same direction) and have the same oscillation amplitude

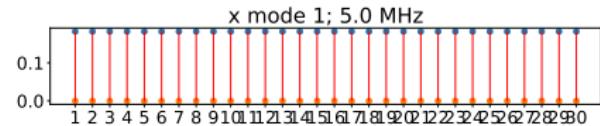


²This follows from the Euler-Lagrange equations.

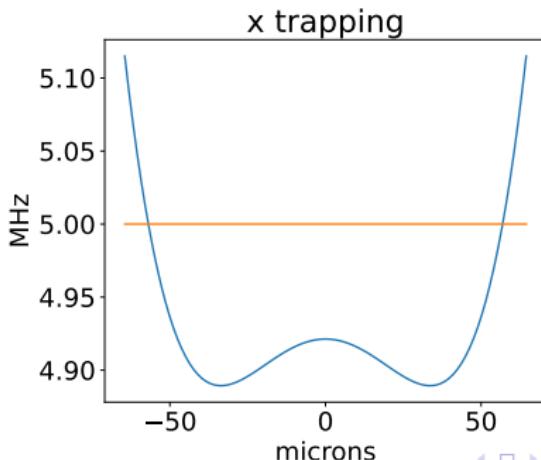
Why poor center of mass modes?



(a) COM mode of U_{blade}



(b) COM mode of U_{target}



Coefficient-level optimization

- Distance: Euclidean norm $L = \|\mathbf{Av} - \boldsymbol{\beta}_{\text{target}}\|$
- Does not work well in practice since all components of $\boldsymbol{\beta}$ are treated equally
- Solution: use weights \mathbf{W} (diagonal matrix),
 $L = \|\mathbf{W}\mathbf{Av} - \mathbf{W}\boldsymbol{\beta}_{\text{target}}\|$

ie instead of $L(u, v) = \|u - v\| = \sqrt{\sum_{i=1}^n (u_i - v_i)^2}$, we now have $L'(u, v) = \sqrt{\sum_{i=1}^n (w_i(u_i - v_i))^2}$

Grid-level optimization

- Previously: β_{blade} vs β_{target}
- Alternative approach: U_{blade} vs U_{target} on a grid
- $U(x, y, z) = \sum_m \beta_m x^i y^j z^k$ implies some matrix \mathbf{E} maps $\boldsymbol{\beta}$ to the values of U on a grid

ie $[\mathbf{E}]_{pm} = x_p^i y_p^j z_p^k$ and

$$[\mathbf{E}\boldsymbol{\beta}]_p = \sum_m [\mathbf{E}]_{pm} [\boldsymbol{\beta}]_m = \sum_m \beta_m x_p^i y_p^j z_p^k = U(x_p, y_p, z_p)$$

- Loss function: $L = \|\mathbf{E}\mathbf{A}\mathbf{v} - \mathbf{E}\boldsymbol{\beta}_{\text{target}}\|$