Read me

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1 Introduction

This is a brief introduction to the documents in the working file, which mainly consist of Matlab programs(end with 'mlx'), Matlab data(end with 'mat'), Markdown draf(end with 'md') and a few references (end with 'pdf'). You can also find some record of the experiment in the OneNote 'SQRLab.one' and only few of the programs have been renamed, while the summary of the summer research is presented in a paper 'Background_gas_collisions.pdf', where most of the ideas in the programs can be found.

2 The programs

Most of the calculation and simulation programs are written in Matlab and they can be sorted as following.

1. To calculate the energy barrier according to the APL by Kim.
'Background_gas_collision_four_ions.mlx' and 'Background_gas_collision_two_ions.mlx' are included. While the latter one also gives the result of estimated reorder probability based on this model.

2. To produce the samples of obeying the Maxwell-Boltzmann distribution
The 'Maxwell_Boltzmann_distribution.mlx' illustrates the speed distribution of H_2 and also produce 1000 samples obeying such distribution. The samples are used in the Monte Carlo simulation.

3. To simulate the dynamics of ions time evolution using Euler method.
The 'draft_on_several_ions.mlx' is a series of codes to simulate different number of ions' in the 2D trap and you can comment out the unnecessary codes and choose the one you need. One detail remarkable is that $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t+\Delta t)\Delta t$ instead of $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \frac{\vec{v}_i(t)+\vec{v}_i(t+\Delta t)}{2}\Delta t$, as the latter one is easier to diverge. And the 'simulation_2_D_3_ions.mlx' is already contained in it.
The 'draft_on_3D_ions.mlx' has the same structure as the 'draft_on_several_ions.mlx' and carries out the simulation for 3D space.

The 'draft_on_4_electrodes_potential.mlx' and 'draft_on_ions_in_pseudopotential.mlx' simulate the ions' dynamics in the pseudo-potential. The latter one is used as the original code for Monte Carlo simulation of ions in the pseudo-potential.

4. The Monte Carlo simulation
It takes around 8h to finish running 1000 samples for simulation.
Part.2 and Part.3 are contained in these programs. Programs begin with 'Monte_Carlo' all belong to Part.4 and the file names already explain their function. The parameter 'n' can be changed for different numbers of samples to simulate. It is noticeable that for 3 ions the 2/3 samples are used to simulate the collision on the side ion and 1/3 on the central ion while for 4 ions 1/2 are used for side collisions and 1/2 for central ones, which actually cut the programs into halves. Thus, when adjusting the total of samples by the parameter 'n', the parameter in the two halves needs to be revised as well, though this shortage has been solved in 'Monte_Carlo_pseudopotential_3ions_simulations.mlx'.

5. The analysis of the result
Matlab data(end with 'mat') need to be load for these programs.
The 'Plot_result.mlx' is used to analyse the result exported from the Part.4 and output the plots of reorder probability. The 'Energy_barrier_2D_calculation.mlx' gives the effective energy barrier for the 2D simulation.

6. The Comparison to the previous APL paper
The 'Potential_plot.mlx' gives an accurate plot of enerngy and the phase space for 2 ions in the 1D harmonic trap while the 'draft_on_poptential.mlx' presents the 2D condition using the rough approximation that one of the ion is static. The 'Model_simpified_Energy_barrier.mlx' calculated the energy difference between the saddle point and the ground state which is close to the APL calculation. And the defect of the APL model is discussed in the summary report.

7. Some python programs
There are a few python programs written with 'numpy' and they work the same as section 2 Part.2 and 3 except for some using the divergent method described in section 2 Part.3.

3 The data

Most data are named according to the corresponding Monte Carlo simulation programs. For the 2D simulation of 3 and 4 ions, the difference between collisions on the side and central ion is also discussed. Important data are 'w1', 'w2' and 'reorder', which mean ω_r, ω_z and the count of reorder in 1000 samples of each trapping frequency. And the data end with 'new' means the 2D collision is taken into consideration while the ones without 'new' simply consider the center-to-center collision.