Development of a Detailed Kinetic Theory for Quadrupole Ion Traps

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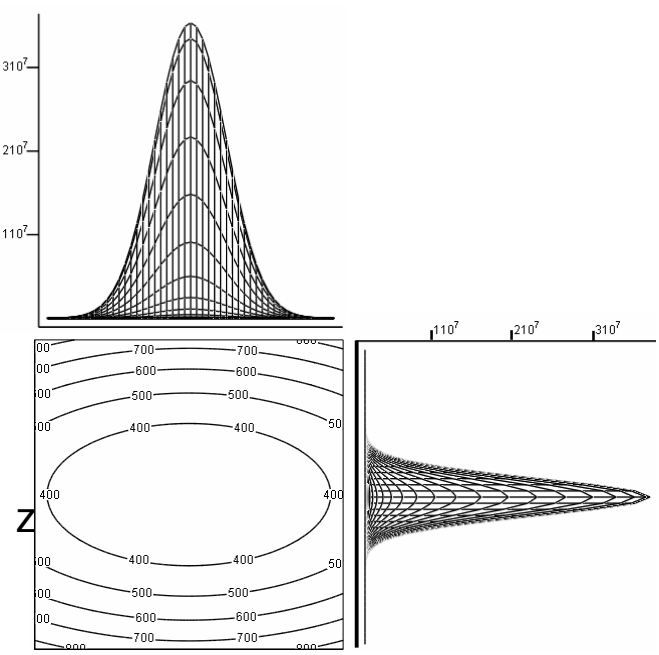
Basic research at the Oak Ridge National Laboratory has led to development of a detailed kinetic theory for quadrupole ion traps, the electrodynamic devices driving mass spectrometers routinely used in studies ranging from the investigation of the fate of small molecule by-products of energy production and consumption to the study of large biomolecules and their complexes. The differential equations incorporated in the theory do not appear to have been given previously, probably because of the difference in viewpoint between this approach, which focuses on average behavior of an ion ensemble, and others, which concentrate on the individual trajectories of single (or multiple) ions. Knowledge gained from the theory is a prerequisite for enhancing such mass spectrometric analysis and characterization methods. At the same time, insights resulting from the knowledge will likely enable accurate manipulation of ion temperatures and internal energies, thereby enhancing the utility of ion traps as a tool for investigating fundamental ion chemistry.

Using numerical methods to solve the equations, which describe the dynamic electric fields and ion-neutral collisions that are integral to ion trap operation, the effect of changes in operating parameters on the position- and time-dependent ion kinetic energy and temperature, as well as the overall number density distribution, can be predicted from first principles. Combining the above information enables metrics for the entire ion ensemble, such as effective temperature, to be determined as a function of time. Because the collisions are treated at the same level of sophistication and detail as is used to deal with the time- and space-dependent electric fields, the theory is not dependent on any special assumptions about the ion-neutral interactions or mass ratio. Furthermore, the kinetic theory for the quadrupole ion trap should be extendable to the linear ion trap, which has all the capabilities of a quadrupole trap while exceeding its performance in other areas.



Effective temperature contours in the axial plane calculated for the quadrupole ion trap. The number density distribution calculated for a population of 10^5 ions is also indicated.

This study is being submitted to the *Journal of Chemical Physics* under a collaboration involving Oak Ridge National Laboratory (FWP ERKCC42) and Chatham College.