Space-charge-limited Coulomb crystals in a 3D Paul trap: direct N-body simulation versus cold-fluid theory

V R Alagappan[1], B Govindan[2] and K T Satyajith[3†]

[1]IISER Tirupati, Jangalapalli, India
[2]Nuclear Design and Engineering, L&T Heavy Engineering, Surat, India-395007
[3]Delta Q, IMJ Institute of Research and Department of Basic Science and Humanities, Moodalkatte Institute of Technology, Moodalkatte, Karnataka 576217, India

Synopsis At fixed static voltage, a cooled Coulomb crystal in a 3D Paul trap flattens as the RF amplitude rises. Direct N-body simulations in the full RF field show its aspect ratio falling from 0.72 to 0.41 between 150 and 250 V, so its radius shrinks as $V_{\rm rf}^{-0.45}$ rather than the fixed-shape $V_{\rm rf}^{-2/3}$. A parameter-free cold-fluid model reproduces the shape to 1.5% and the radius to 1% at $N = 1000$.

Once Coulomb repulsion balances the trapping field, cold-fluid theory predicts the size and shape of a cooled ion cloud from the trap parameters alone [1]. Earlier tests compared crystal shapes with experiment and ion numbers with molecular dynamics [2]; here we test the absolute radius, aspect ratio and density against direct N-body simulations in the full RF field.

We integrate every ion in the instantaneous field of an ideal 3D quadrupole trap ($r_0 = 1$ mm, $\Omega/2\pi = 10$ MHz, $U_{\rm dc} = 5$ V), with exact Coulomb forces and no pseudopotential approximation. A Langevin thermostat [3] at the $^{40}Ca^{+}$ Doppler limit represents laser cooling. Clouds of $N = 10$–1000 ions start at rest at $V_{\rm rf} = 150$–300 V ($q_z = 0.37$–0.73).

At $V_{\rm rf} \leq 250$ V every cloud relaxes within a few microseconds into an oblate Coulomb crystal below 0.8 mK, with $R_{\rm rms} \propto N^{0.352\pm0.004}$ (Fig. 1a).

The cold-fluid model combines the uniform density $n_0 = 3\varepsilon_0 V_{\rm rf}^2/(m\Omega^2 r_0^4)$, the spheroid shape set by the depolarisation factor [1], and RF-averaged micromotion. With no free parameters it reproduces the radius to 10% at $N = 10$ and 1% at $N = 1000$; the residual is a $V_{\rm rf}$-independent density excess of the discrete crystals (5% at $N = 200$, 1.5% at $N = 1000$).

At fixed $N = 200$ the density rises as $V_{\rm rf}^2$, but because the static voltage makes ω_z/ω_r grow with $V_{\rm rf}$, the crystal also flattens. Its measured aspect ratio falls from 0.72 to 0.41 between 150 and 250 V, within 1.5% of the model (Fig. 1b). The radius therefore falls as $V_{\rm rf}^{-0.45}$ (21.6 to 17.2 μm, within 2%), not as the fixed-shape $V_{\rm rf}^{-2/3}$. Exact Floquet secular frequencies, used instead, overestimate both.

At 300 V ($q_z = 0.73$), a cloud released from the initial distribution did not crystallise, whereas a pre-formed crystal remained cold. We are investigating the origin of this dependence on the initial state.

The flattening can be imaged directly, and the results set a baseline for space-charge frequency shifts and mixed-species crystals.

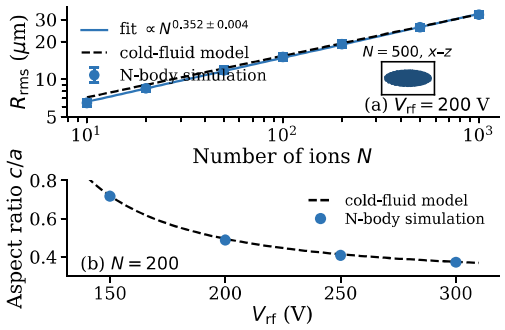

Figure 1. (a) $R_{\rm rms}$ vs N, 200 V (inset: $N = 500$). (b) Aspect ratio vs $V_{\rm rf}$, $N = 200$.

Framework co-developed with Princita Gazel Ferrao, Vandana and Vedha Varshini B [4].

References

[1] Dubin D H E and O'Neil T M 1999 *Rev. Mod. Phys.* **71** 87
[2] Fröhlich U, Roth B and Schiller S 2005 *Phys. Plasmas* **12** 073506
[3] Schneider T and Stoll E 1978 *Phys. Rev. B* **17** 1302
[4] Alagappan V R *et al.* in preparation

†E-mail: ktsatyajit@proton.me