From electrode asymmetry to octupole anharmonicity: quantum motional dynamics of a single ion in a Paul trap

S Jana[1†], A Dey[1], P Mandal[2] and N Deb[1†]

[1]School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata 700032, India
[2]Department of Physics, St. Paul's Cathedral Mission College, Kolkata-700009, India

Synopsis Radial diagonal asymmetry in round-rod quadrupole devices generates octupole fields that are absent in the symmetric geometry. Building on our earlier SIMION studies of these fields, we treat the resulting quartic anharmonicity quantum mechanically for a single ion in an RF Paul trap. The octupole term opens $\Delta n = \pm 4$ channels and adds occupation-dependent phase shifts: the phonon-number variance rises by ∼18% against ∼6% for the mean, while RF-generated quadrature squeezing survives but is weakened and reoriented.

In symmetric round-rod traps only dodecapole and icosapole harmonics accompany the quadrupole field, but any radial asymmetry breaks the fourfold symmetry. Using SIMION simulations, we showed that changing the radius of a single rod [1], or displacing or resizing a diagonal rod pair [2], generates octupole (A_4) and hexadecapole (A_8) components that grow with the asymmetry parameter γ (Fig. 1a). Classically, they shift the stability apex, broaden the transmission contour and degrade the resolution in step with $|A_4| + |A_6|$ [1, 2]. The octupole is thus the leading, practically unavoidable, anharmonic correction to the trapping field.

Here we ask what it does to the *quantized* ion motion. We retain the full RF time dependence, $V = (m\Omega^2/8)(a + 2q\cos\Omega t)(x^2 + \lambda x^4)$ with $\lambda = A_4/r_0^2$, and work in the Fock basis of a reference oscillator, $\omega_0 = \sqrt{a}\,\Omega/2$. The quadratic RF term couples $\Delta n = \pm 2$ and squeezes; the quartic term adds $\Delta n = \pm 4$ couplings and a Kerr-like diagonal shift $\propto 6n^2 + 6n + 3$. Parity conservation confines an initial vacuum to the even ladder. The Schrödinger equation ($N = 80$, converged to $N = 120$) is integrated over 1000 RF cycles at $a = 0.1$, $q = 0.5$ for $\lambda = A_4\ell_\Omega^2/r_0^2 \le 5 \times 10^{-4}$, $\ell_\Omega = \sqrt{\hbar/m\Omega}$.

The octupole builds a weak, converged population tail up to $n \approx 80$. Since $\langle n^2\rangle$ weights it by n^2, the cycle-averaged variance rises from 1.59 to 1.88 while $\langle n\rangle$ moves only from 0.485 to 0.515; the Mandel parameter grows from 2.27, already large from RF pair creation, to 2.65. Quadrature squeezing is robust: $S_{\min} < 0$ at every RF phase of the 1000th cycle, with $(\Delta X_s)^2 = 0.102$ versus 0.086 without the octupole (vacuum 0.5). It is, however, reduced and reoriented (Fig. 1b), as n-dependent phases dephase $\langle \hat{a}^2\rangle = \sum_n \sqrt{(n+1)(n+2)}\, c_n^* c_{n+2}$.

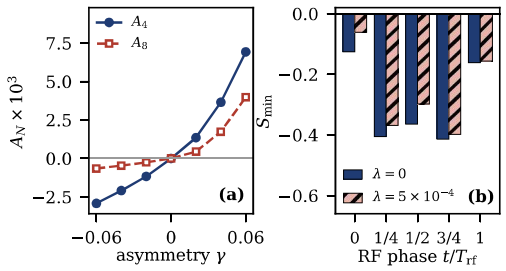

Figure 1. (a) Octupole (A_4) and hexadecapole (A_8) coefficients versus single-rod asymmetry γ ($\eta = 1.14$) [1]. (b) Minimum squeezing parameter $S_{\min}$ at five phases of the 1000th RF cycle ($a = 0.1$, $q = 0.5$).

Number and quadrature fluctuations thus respond oppositely to the same perturbation (Fock-space spreading versus phase-space shearing), linking the multipole analysis of imperfect traps [1, 2] to nonclassical motional-state control [3].

References

[1] Jana S *et al.* 2025 *Int. J. Mass Spectrom.* **517** 117495
[2] Jana S *et al.* 2025 *J. Am. Soc. Mass Spectrom.* **37** 180-187
[3] Leibfried D *et al.* 2003 *Rev. Mod. Phys.* **75** 281

†E-mail: sukanya03jana@gmail.com
†E-mail: nabanita.deb@iacs.res.in