Nonresonant averaging of an inhomogeneous nonlinear Mathieu equation

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Abstract. An ion in a Paul trap obeys the Mathieu equation. An added DC dipolar field in a quadrupole ion trap adds a constant and a small quadratic term to the governing equation. We examine the resulting dynamics with light damping using second-order averaging. For the unperturbed equation, i.e., the linear inhomogeneous Mathieu equation, we use Fourier series instead of Mathieu functions. We do not focus on specific resonances and consider general nonresonant conditions. Slow flows, obtained after manipulating rather long Fourier series expansions, offer a very good match with the full equation. Phase portraits of the slow flow show that a basic periodic solution, found separately using harmonic balance, is generally stable. Practical trap operation involves parameter values where the perturbation approximation stuggles a bit, but still works. Satisfactory insights into trap operation are obtained.

Introduction

Traditional ion trap mass spectrometers have two endcaps and a ring electrode. When the endcaps are grounded and AC excitation is given to the ring electrode, axial motions obey the Mathieu equation. An added dipolar DC excitation across the endcaps is used for collision induced dissociation, or breaking large ions into smaller fragments. An early treatment of such excitation was given by Plass [1] using Mathieu functions and a constant added term. Here we use a simpler basic solution and include a small quadratic term that is actually present under DC excitation. In particular, we study

$$\zeta'' + \varepsilon^2 \eta \zeta' - 2q \cos(2\xi) \zeta = \mu \left(1 + \varepsilon \zeta^2\right),\tag{1}$$

where the prime (') denotes differentiation with respect to nondimensional time ξ ; and where ζ , η , q and μ are nondimensional and represent ion displacement, damping, AC quadrupole and DC dipolar excitations, respectively. Earlier, Abraham and Chatterjee [2] used harmonic balance in averaging to study a weakly nonlinear homogeneous Mathieu equation near resonances. Here we allow an inhomogeneous term and general q.

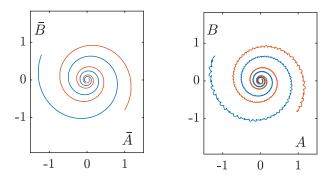


Figure 1: Comparison of phase portraits obtained from Eq. (1): slow flow (left) and full numerics (right).

Results and discussion

We first consider a general solution $\zeta = A\phi_1(\xi) + B\phi_2(\xi) + \chi(\xi)$ of a linear Mathieu equation with a constant right hand side. We approximate ϕ_1 , ϕ_2 and χ using several terms in harmonic balance approximations. We also numerically approximate q as a simple function of β , which is left as a free parameter. Second order averaging yields slow flow equations for the amplitudes $\overline{A}(\xi)$ and $\overline{B}(\xi)$, which agree well with full solutions of Eq. (1) (Fig. 1). The coefficients in the slow flow show stability of the origin in the averaged phase portrait, indicating stability of χ for general β . This stability result for the general nonresonant case, the nature and size of χ , as well as some simple further approximations for χ itself, can be useful for practical operations of the trap under dipolar excitation.

References

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