Comment on "Regular and chaotic motions in ion traps: A nonlinear analysis of trap equations"

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In a recent publication Baumann and Nonnenmacher [Phys. Rev. A **46**, 2682 (1992)] analyze the equations of motion of two ions in a Paul trap in the pseudopotential approximation. Chaos and nonzero Liapunov exponents are found for trap asymmetry parameter $\lambda=\frac{1}{2}$ and angular-momentum parameter $\nu\neq 0$. It is pointed out that besides the total energy E, a constant of the motion, $G=[\nu^2/\rho+\rho\dot{\zeta}^2-\dot{\rho}\zeta\dot{\zeta}+\rho/(\rho^2+\zeta^2)^{1/2}-\zeta^2\rho/4]^2+\nu^2(\rho\dot{\rho}+\zeta\dot{\zeta})^2/\rho^2+\nu^2(\rho^2+\zeta^2)$, exists for $\lambda=\frac{1}{2}$ and arbitrary ν. Therefore, and contrary to the claims by Baumann and Nonnenmacher, chaos cannot exist for $\lambda=\frac{1}{2}$, and the Liapunov exponents are expected to be zero.

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With the help of analytical techniques and supported by detailed numerical calculations Baumann and Nonnenmacher [1] recently analyzed the equations of motion of two ions in a Paul trap. The Hamiltonian used to describe the ion motion was derived by a Landau-Kapitza averaging technique [2] (the pseudopotential approximation) and is given by [1,3]

$$H=\tfrac{1}{2}(p_\rho^2+p_\zeta^2)+\tfrac{1}{2}(\rho^2+\lambda^2\zeta^2)+\frac{1}{[\rho^2+\zeta^2]^{1/2}}+\frac{\nu^2}{2\rho^2} . \quad (1)$$

Here ρ refers to the separation of the two ions in the x-y plane of the trap, ζ is their separation in z direction, and $p_\rho=\dot{\rho}$, and $p_\zeta=\dot{\zeta}$ are the corresponding momenta. The asymmetry parameter $\lambda=\omega_z/\omega_\rho$ is defined as the ratio of the secular frequencies of the trap in z and ρ direction, respectively, and ν is proportional to the z component of the angular momentum of the two ions. The equations of motion derived from (1) are given by [1,3]

$$\ddot{\rho}=\frac{\rho}{(\rho^2+\zeta^2)^{3/2}}-\rho+\frac{\nu^2}{\rho^3} , \quad (2a)$$

$$\ddot{\zeta}=\frac{\zeta}{(\rho^2+\zeta^2)^{3/2}}-\lambda^2\zeta . \quad (2b)$$

According to current knowledge [1,3] and due to the nonlinear nature of (1) the equations of motion (2) possess mostly chaotic solutions and are integrable only for special values of λ and associated special values or ranges of ν, respectively. For $\lambda=2$, for instance, a constant of the motion F exists [1,3] which is given by

$$F(\rho,\dot{\rho},\zeta,\dot{\zeta};\nu)=\zeta\dot{\rho}^2-\dot{\zeta}\rho\dot{\rho}+\frac{\zeta}{(\rho^2+\zeta^2)^{1/2}}-\rho^2\zeta+\frac{\nu^2\zeta}{\rho^2} . \quad (3)$$

Using a generalized Runge-Lenz vector, the constant F was first derived in Ref. [3]. Its analytical form, however, was not stated correctly in Ref. [3]; a factor ζ is missing in the second term of Eq. (36) in Ref. [3]. The constant F was correctly stated in Ref. [1]. For $\lambda=\frac{1}{2}$ a constant of the motion G can be derived from the length of the generalized Runge-Lenz vector [3],

$$G(\rho,\dot{\rho},\zeta,\dot{\zeta};\nu)=I_\rho^2+I_\phi^2+\nu^2(\rho^2+\zeta^2) , \quad (4a)$$

with

$$I_\rho=\frac{\nu^2}{\rho}+\rho\dot{\zeta}^2-\dot{\rho}\zeta\dot{\zeta}+\frac{\rho}{(\rho^2+\zeta^2)^{1/2}}-\tfrac{1}{4}\zeta^2\rho \quad (4b)$$

and

$$I_\phi=-\frac{\nu}{\rho}(\rho\dot{\rho}+\zeta\dot{\zeta}) . \quad (4c)$$

Unfortunately, I_ρ was not reported correctly in Ref. [3], for which the author apologizes. That G, as defined in (4), is indeed conserved can be checked immediately by calculating dG/dt and using the equations of motion (2).

As a consequence, the equations of motion (2) are integrable for $\lambda=\frac{1}{2}$ and arbitrary ν. This is so because in addition to G the total energy E is a conserved quantity and the phase space of the two-ion problem as defined in (1) is four dimensional. On the basis of this result, regular motion and zero Liapunov exponents are expected for $\lambda=\frac{1}{2}$ and arbitrary ν.

Baumann and Nonnenmacher devote three figures of their paper to convince the reader of the existence of chaos for $\lambda=\frac{1}{2}$ and $\nu\neq 0$. In Fig. 4, Ref. [1], a nonzero Liapunov exponent is shown for $E=1.8$, $\lambda=\frac{1}{2}$, and $\nu=\frac{1}{10}$. Because of the simultaneous existence of E and G this result is surprising. Global exponential divergence of nearby trajectories in an integrable system may be possible for an open system but since the available phase space of the two-ion system (1) at constant energy is confined (compact) the appearance of a nonzero Liapunov exponent in this integrable situation cannot be understood.

In Fig. 5, Ref. [1], a Poincaré section is shown for $\lambda=\frac{1}{2}$ and $\nu=\frac{1}{10}$ which corresponds to Fig. 4, Ref. [1]. This Poincaré section is interpreted as showing a chaotic situation. On the other hand, the complicated appearance of Fig. 5 may be due to numerical problems. Howard and Farrelly have recently calculated Poincaré sections for the parameters used in Fig. 5 and saw only invariant curves [4]. This result is perfectly consistent with the simultaneous existence of E and G for $\lambda=\frac{1}{2}$.

Figure 6, Ref. [1], finally, shows a spectrum of maximal Liapunov exponents for $\lambda=\frac{1}{2}$ as a function of ν. The Liapunov exponents are shown to be nonzero for four different energies and ν ranging from 0 to 1. But since G exists for all ν, and the phase space is compact, the Liapunov exponents are expected to be zero in this case. Therefore, the nonzero result reported in Fig. 6, Ref. [1], is very surprising. It is possible that the authors stopped the integration of the equations of motion too early when calculating the Liapunov exponents.

Nontrivially integrable Hamiltonian systems, such as (1) for $\lambda=\frac{1}{2}$, are very rare in the physics literature. Therefore, the Hamiltonian (1), which additionally bears some resemblance to the problem of a hydrogen atom in a generalized van der Waals potential [4–7], may deserve some further attention.

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