COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in the **Physical Review**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

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

David Farrelly and James E. Howard
Department of Chemistry and Biochemistry, Utah State University, Logan, Utah 84322-0300
(Received 8 October 1992)

Using Lie-group and prolongation techniques, Baumann and Nonnenmacher [Phys. Rev. A **46**, 2682 (1992)] recently studied integrability of a Hamiltonian describing the dynamics of ion traps. It is pointed out that their results can be obtained more simply and directly by recognizing that the problem is separable in each of the integrable limits found by Baumann and Nonnenmacher. Similarities between this system and a hydrogen atom in a generalized van der Waals potential are also considered.

PACS number(s): 32.80.Pj, 02.20.−a, 02.60.−x, 35.10.−d

In a recent paper Baumann and Nonnenmacher [1] studied the dynamics of two ions in a Penning or Paul trap. Using Lie-group methods they determined exact integrals of the motion in various limits, all of which had been discovered previously by Blümel *et al.* [2]. This approach was prompted by a failure of the Painlevé test to uncover global integrals of the motion. The purpose of this Comment is twofold: First, to remark that the existence of these integrals is a simple consequence of the separability of the problem in appropriate coordinates, and second, to comment on the classical dynamical simulations presented in [1].

In cylindrical coordinates (ρ,ζ) the Hamiltonian studied in [1] is

$$H=E=\tfrac{1}{2}(P_\rho^2+P_\zeta^2)+\tfrac{1}{2}(\rho^2+\lambda^2\zeta^2)+\frac{1}{r}+\frac{\nu^2}{2\rho^2}\ , \qquad (1)$$

where $r=(\rho^2+\zeta^2)^{1/2}$, and λ and ν are dimensionless physical control parameters. It is illuminating to compare the ion-trap Hamiltonian (1) with that of a hydrogen atom in a generalized van der Waals potential (GVDW) [3–5]. In Cartesian coordinates the GVDW Hamiltonian is

$$H'=\tfrac{1}{2}(P_x^2+P_y^2+P_z^2)+\frac{\gamma}{2}(x^2+y^2+\lambda^2z^2)-\frac{1}{r}\ , \qquad (2)$$

where γ and λ are again dimensionless physical parameters. Scaling the coordinates by $\gamma^{-1/3}$ and the momenta by $\gamma^{1/6}$ and going to cylindrical coordinates ($x=\rho\cos\phi$, $y=\rho\sin\phi$, $z=\zeta$) gives the Hamiltonian

$$K=\gamma^{-1/3}H'=\tfrac{1}{2}(P_\rho^2+P_\zeta^2)+\tfrac{1}{2}(\rho^2+\lambda^2\zeta^2)-\frac{1}{r}+\frac{m^2}{2\rho^2}\ . \qquad (3)$$

Equation (3) is identical to Eq. (1) except for the sign of the Coulomb term. Thus the analysis presented here for the ion trap applies equally to the GVDW system. In both cases the system is seen to consist of a two-dimensional oscillator plus Coulomb and centrifugal terms. Importantly, the z component of angular momentum (L_z) is an exact constant of motion of (1) and (3); in the ion-trap problem it is related to ν while in the GVDW system it corresponds to the magnetic quantum number m.

In what coordinate systems, if any, is Eq. (1) separable? The Coulomb problem is well known to be separable in both polar and parabolic coordinates [6]. The oscillator contribution to H is clearly separable as written in cylindrical coordinates. In addition, the oscillator may separate in other coordinate systems when the frequencies in the two modes are commensurate (i.e., a ratio of integers). [The frequencies in the oscillator modes will be denoted by $\omega_\rho=1$ and ω_ζ (*alias* $|\lambda|$).] Specifically, when $\omega_\rho{:}\omega_\zeta$ stand in a 1:1 ratio ($\lambda=\pm1$) the two-dimensional oscillator is also separable in polar coordinates while in the cases of 1:2 ($\lambda=\pm2$) or 2:1 ($\lambda=\pm\frac{1}{2}$) frequency ratios it is separable in parabolic coordinates [7]. The complete Hamiltonian (1) can therefore be expected to separate when the oscillator portion together with the Coulomb and centrifugal terms are all separable in the same coordinate system.

When $\lambda=\pm1$ the Hamiltonian (1) is separable in spherical polar coordinates. To see this, the Hamiltonian (1) with $\lambda=\pm1$ is first converted to Cartesian coordinates giving

$$H=\tfrac{1}{2}(P_x^2+P_y^2+P_z^2)+\tfrac{1}{2}(x^2+y^2+z^2)+\frac{1}{r}\ , \qquad (4)$$

where ν does not now appear explicitly. It is apparent

that Eq. (4) is separable in spherical polar coordinates (for arbitrary ν) and reduces to a radial equation. Similar considerations apply to the GVDW problem.

For a 1:2 frequency ratio ($\lambda=\pm 2$) the transformation to parabolic coordinates,

$$\xi=(u^2-v^2)/2, \quad \rho=uv \ , \tag{5}$$

leads to a complete separation for arbitrary ν. In these coordinates Eq. (1) becomes

$$H=\frac{1}{2(u^2+v^2)}\left[P_u^2+P_v^2+u^6+v^6+4+\frac{\nu^2(u^2+v^2)}{u^2v^2}\right], \tag{6}$$

and the Hamilton-Jacobi equation is separable upon multiplication by (u^2+v^2). Similarly, the GVDW problem also separates in this coordinate system as noted in Ref. [4].

In the case of a 2:1 ratio of frequencies ($\lambda=\pm\frac{1}{2}$) the system might again be expected to separate using a different set of parabolic coordinates,

$$\rho=(u^2-v^2)/2, \quad \xi=uv \ , \tag{7}$$

which yields

$$H=\frac{1}{2(u^2+v^2)}\left[P_u^2+P_v^2+\frac{u^6}{4}+\frac{v^6}{4}+4\right]+\frac{2\nu^2}{(u^2-v^2)^2} \ . \tag{8}$$

The term in ν^2 in the Hamiltonian obviously prevents complete separability. Hence the problem separates only when $\nu=0$ for $\lambda=\pm\frac{1}{2}$, so that the integral obtained upon separation is valid only in the limit that $\nu=0$. This agrees with [1] where an integral was found for $\nu=0$ with $\lambda=\pm\frac{1}{2}$. The integrals of motion when the problem is separable in parabolic coordinates are closely related to the Runge-Lenz vector of the Coulomb problem [3–6]. In fact, the Runge Lenz vector is essentially the separation constant in parabolic coordinates [6].

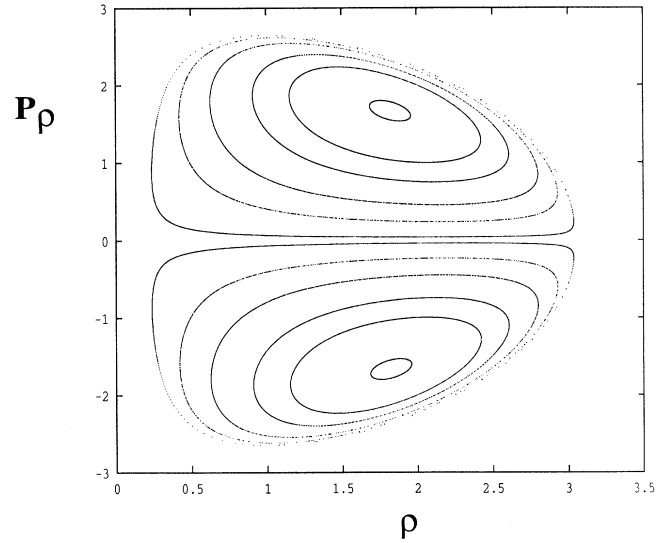

FIG. 1. Poincaré surface of section in the (P_ρ,ρ) plane for several sets of initial conditions with $E=5$, $\lambda=2$, and $\nu=0$. These parameters correspond to Fig. 2 of [1].

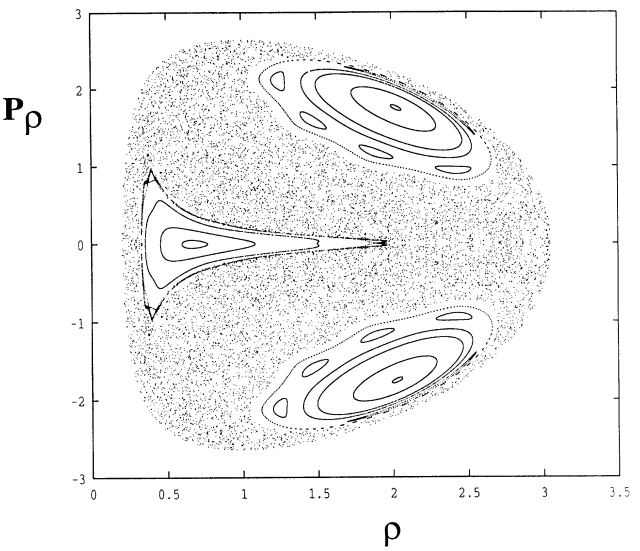

FIG. 2. As Fig. 1 but for $\lambda=2.1$, corresponding to Fig. 3 of [1].

The case $\lambda=\pm\frac{1}{2}$ and arbitrary ν was treated by Blümel *et al.* [2], who derived a global invariant $G(\rho,\xi,P_\rho,P_\xi)$ by means of a generalized Runge-Lenz vector. The reader is cautioned, however, that Eqs. (31)–(38) of [2] contain algebraic errors [8]. In corrected form, Eq. (37) of [2] does indeed give a valid global invariant, so that (1) is integrable for $\lambda=\pm\frac{1}{2}$ and arbitrary ν. This integral of motion does not seem to be related in any obvious way to further separability of (1).

The Poincaré surfaces of section presented in [1] are somewhat puzzling. Specifically, in Figs. 2 and 5 of [1] the Kol'mogorov-Arnol'd-Moser (KAM) curves associat-

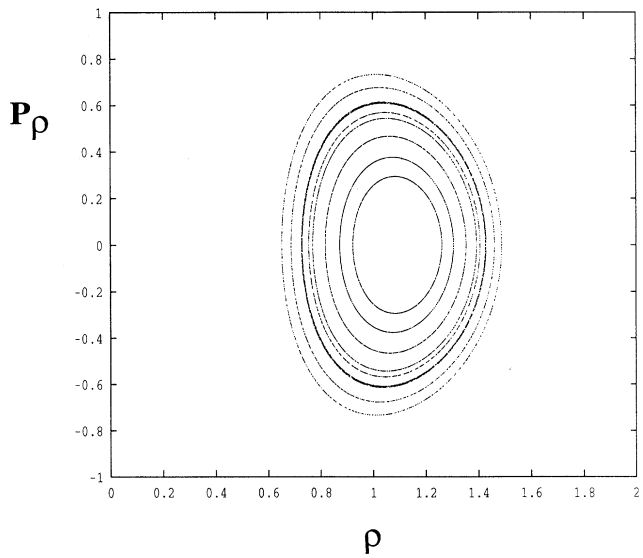

FIG. 3. As Fig. 1 but for $E=1.8$, $\lambda=0.5$, and $\nu=0.1$, corresponding to Fig. 5 of [1].

ed with a single trajectory cross each other multiple times. This is a result of failing to select a single branch of the Hamiltonian when projecting the dynamics onto the surface of section [9]. We present surfaces of section in Figs. 1 and 2 in the (P_ρ,ρ) plane defined by $\zeta=0$ and $P_\zeta>0$. Figures 1 and 2 correspond to Figs. 2 and 3 of [1] except that several different sets of initial conditions are integrated. The results in these two cases agree with the *general* conclusions contained in [1] concerning integrability of the dynamics, i.e., chaotic versus regular motion. However, our definition of the surface of section does not give rise to crossings of KAM curves. Figure 3 is a section computed with $\lambda=\pm\frac{1}{2}$ and ν nonzero and is chosen to correspond to Fig. 5 of [1]. While the equivalent section in [1] exhibits chaotic dynamics we could find no evidence of chaos for this set of parameter values. We have established numerically that the chaos apparently generated by a single trajectory in Fig. [5] of [1] is *not* due to the particular choice of section made in [1]. We can only conclude that the chaos in Fig. [5] of [1] is a result of numerical error and is therefore spurious. This, in turn, would affect the calculation of Lyapunov exponents presented in Fig. 4 of [1]. An extensive search in which the energy and ν were varied over a wide range of values similarly failed to find any evidence of chaos for $\lambda=\pm\frac{1}{2}$. Therefore, our calculations support the existence of a global invariant for $\lambda=\pm\frac{1}{2}$ and ν arbitrary [2,8].

An obvious way to search for additional integrals of motion is the Painlevé test [10]. However, Baumann and Nonnenmacher [1] report (without providing details) that the Painlevé test failed to uncover *any* integrals of motion for the ion-trap problem. In contrast, for the GVDW problem, Ganesan and Lakshmann [4] were able to discover integrals of the motion using the Painlevé test in parabolic coordinates: For $m=0$ and arbitrary γ they found the problem to be integrable when $\lambda=1$, 2, and $\frac{1}{2}$. These results correspond to the results for the ion-trap problem with $\nu=0$. The similarity between the two Hamiltonians and the apparent disparity in the applicability of the Painlevé test suggests that further analysis would be profitable.

In conclusion, we note that in *all* cases the integrals discovered in [1] and [4] can be recovered using separability of the system in the appropriate coordinate system. The remarkable separability discovered here has been previously overlooked in both the ion-trap and the GVDW problem [1–5].

Note added in proof. Since the submission of this Comment we have discovered a paper by A. Deprit and S. Ferrer [Phys. Lett. A **148**, 412 (1991)] that points out that the GVDW system separates for $\lambda=\pm2,\pm\frac{1}{2}$ in the case that $m=0$.

We acknowledge useful conversations with R. Blümel and J. D. Meiss. Financial support by a grant from the Petroleum Research Fund, administered by the American Chemical Society is gratefully acknowledged.

[1] G. Baumann and T. F. Nonnenmacher, Phys. Rev. A **46**, 2682 (1992).

[2] R. Blümel, C. Kappler, W. Quint, and H. Walther, Phys. Rev. A **40**, 808 (1989); **46**, 8034(E) (1993).

[3] Y. Alhassid, E. A. Hinds, and D. Meschede, Phys. Rev. Lett. **59**, 1545 (1987).

[4] K. Ganesan and M. Lakshmann, Phys. Rev. Lett. **62**, 232 (1989); Phys. Rev. A **42**, 3940 (1990); *ibid.* **45**, 1548 (1992).

[5] J. A. Milligan and D. Farrelly, Phys. Rev. A **47**, 3137 (1993).

[6] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics,* 3rd ed. (Pergamon, Oxford, 1977), pp. 117–132; M. Born, *Mechanics of the Atom,* translated by J. W. Fisher (republished by Ungar, New York, 1960), pp. 212–220.

[7] D. W. Noid, M. L. Koszykowski, and R. A. Marcus, J. Chem. Phys. **71**, 2864 (1979).

[8] R. Blümel (private communication).

[9] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer-Verlag, New York, 1983), Chap. 1; D. K. Arrowsmith and C. M. Place, *An Introduction to Dynamical Systems* (Cambridge University Press, Cambridge, England, 1990), Chap. 1.

[10] Y. F. Chang, M. Tabor, and J. Weiss, J. Math. Phys. **23**, 531 (1982).