Comment on ''Saddle-point ionization and the Runge-Lenz invariant''

David Farrelly
Department of Chemistry and Biochemistry, Utah State University, Logan, Utah 84322-0300
(Received 18 August 1995)

Arguments made recently by Howard [Phys. Rev. A **51**, 3934 (1995)] as to (i) the consequences of the nonexistence of an effective potential in the problem of a hydrogen atom in a circularly polarized microwave field, and (ii) the claimed advantages of his stability analysis as compared to methods based on harmonic expansion at an equilibrium point are examined. [S1050-2947(97)04911-6]

PACS number(s): 32.80.Rm, 42.50.Hz

In a recent article, Howard [1] examined the well-known connection between the Runge-Lenz invariant and the Stark effect for a hydrogen atom: one of the classic problems of fledgling quantum mechanics [2]. This Comment examines a number of specific issues raised in [1] that need to be addressed because they concern problems of current experimental and theoretical interest.

In his study, Howard considered both the Stark effect [3] and the more complicated problem of ionization of hydrogen atoms by circularly polarized (CP) microwave fields, a system that has recently attracted the attention of several researchers [4–7]. A key point of Ref. [1] is that, in the CP problem, it is not possible to define an effective potential: this conclusion led Howard to ''call into question'' (Ref. [1], p. 3944) the validity of previous studies of the CP problem by Nauenberg [4] and by Rzazewski and Piraux [6] who explicitly studied ionization using a potential energy function that is actually equivalent to a zero-velocity surface. Implicitly Howard seems to equate the term *effective potential* with a zero-velocity surface (ZVS) in the sense of celestial mechanics [8–13] (Ref. [1], p. 3936). By extension, other recent research making use of zero-velocity surfaces in this problem (e.g., [7]) must similarly be called into question if Howard's arguments hold water. The sole basis for Howard's questioning is that an effective potential cannot be constructed for the CP problem. This Comment goes over the arguments made by Howard [1].

I. EXISTENCE OF A ZERO-VELOCITY SURFACE

In cylindrical coordinates the CP Hamiltonian (in the planar limit considered in Ref. [1]) is given by

$$H=\frac{1}{2}p_\rho^2+\frac{p_\phi^2}{2\rho^2}-\frac{1}{\rho}-\omega p_\phi+F\rho\cos\phi, \tag{1}$$

where ω and F are the frequency and strength of the microwave field. Howard argues that, because p_ϕ is not conserved, it is impossible to define an effective potential because the kinetic energy is not positive definite. Hence stability cannot be deduced from an effective potential since such a potential does not exist. Following this line of reasoning, Howard then goes on to challenge the findings of researchers who employed a *zero-velocity surface* to examine stability. At this point it is worth emphasizing that the ZVS was invented *precisely* to treat problems for which the kinetic energy is not positive definite [13]. Accordingly, using methods from celestial mechanics [8–12], it is possible to show that not only can a ZVS be defined, but that this potential exhibits both a saddle point and a maximum, making it a legitimate and, indeed, an excellent candidate for the saddle-point analyses performed in Refs. [6,7,14].

In Cartesian coordinates and atomic units the planar CP Hamiltonian is

$$H=E=\frac{1}{2}(p_x^2+p_y^2)-\frac{1}{r}+F[x\cos\omega t+y\sin\omega t]. \tag{2}$$

The explicit time dependence may be removed by transforming to a synodic frame (x',y') rotating with angular velocity ω yielding the Hamiltonian

$$K=\frac{1}{2}(p_x^2+p_y^2)-\frac{1}{r}-\omega(xp_y-yp_x)+Fx \tag{3}$$

and the primes have been dropped. Although the mixing of coordinates with momenta precludes the construction of a potential energy surface in the usual sense, it is possible, in time-honored fashion [8–11], to compute zero-velocity curves which constitute the potential [4]

$$V(x,y)=K-\frac{1}{2}(\dot{x}^2+\dot{y}^2)=-\frac{1}{r}-\frac{\omega^2(x^2+y^2)}{2}+Fx, \tag{4}$$

where $\dot{x}=p_z+\omega y$ and $\dot{y}=p_y-\omega x$. The potential V has critical (equilibrium) points at $y=0$ with x being given by the solutions of the cubic $\omega^2x^3-Fx^2\pm1=0$. Further details may be found in [7]. In fact, Rzazewski and Piraux [6] examined what amount to zero-velocity curves to explain ionization of circular Rydberg states in CP microwave fields using a criterion based on the location of the saddle point: it appears that Howard's claim that this work is incorrect must itself be faulted [14–16].

II. STABILITY OF THE MAXIMUM AND THE KREIN COLLISION

The CP hydrogenic problem is evidently the first problem to be recognized in atomic physics that exhibits a transition from stable to unstable motion at a potential maximum. In this it is similar to the well-known Brown or Trojan bifurcation of celestial mechanics [17], as pointed out recently in two separate papers [7,18]. Howard [1] applies standard variational methods of Hamiltonian stability theory [17] to determine the critical field at which an equilibrium point of the flow destabilizes through a Krein collision. Howard argues that his approach is free of the approximations used in the analysis of Bialynicki-Birula, Kaliński, and Eberly [18]. Actually, the method advocated by Howard is equivalent to the procedure used in Ref. [18]: those authors (i) located the maximum in the ZVS and (ii) performed a stability analysis based on a locally harmonic expansion at the equilibrium point.

It is unclear why Howard states that he obtains ''rigorous stability criteria,'' free of the ''simplifying approximations'' that he implies are introduced by Bialynicki-Birula, Kaliński, and Eberly [18]. In the same vein, Howard made similar claims in an earlier treatment of the stability of the five equilibria of the three-body problem itself [19] (the approach in [1] is evidently derived from this paper): the parallels are obvious and shed light on the issue at hand. In particular, Howard's analysis in [19] should be compared with the much earlier work of Roth [20], Deprit and Deprit-Bartolomé [21], Deprit and Henrard [22], and also Abraham and Marsden [17], all of whom obtain satisfactory descriptions of the stability of equilibria in a similar manner to Ref. [18]. In point of fact, these earlier studies in celestial mechanics inspired the treatment in Refs. [7,18] and constitute accepted and theoretically sound approaches to the problem.

Contrary to the claims of Howard: (i) a compelling picture of saddle-point ionization in the hydrogenic CP problem can be painted using a potential energy that is a ZVS, and (ii) the common approach presented by Farrelly, Lee, and Uzer and by Bialynicki-Birula, Kaliński, and Eberly [7,18,23,24] is no more approximate than the linear stability method used by Howard. Finally, it is worth noting that Ref. [3] discusses in some detail the relationship between the Runge-Lenz invariant (essentially the separation constant in parabolic coordinates, as identified by Epstein and Schwarzschild in 1916 [25]) and the existence of sub-barrier and super-barrier resonant states in the Stark effect, supporting this discussion with extensive semiclassical and quantal calculations of complex energy eigenvalues. Further, Ref. [26] extends the discussion of the connection of the Runge-Lenz invariant to integrability and separability in perturbed Keplerian problems. As aptly noted by Howard in the opening sentence of his paper [1], the ionization of Rydberg atoms by external fields continues to stimulate lively debate.

This work was supported, in part, by a grant from the Petroleum Research Fund, administered by the American Chemical Society, and the National Science Foundation.

[1] J. E. Howard, Phys. Rev. A **51**, 3934 (1995).
[2] M. Born, *The Mechanics of the Atom* (republished by Ungar, New York, 1960) (translated by J. W. Fisher).
[3] D. Farrelly and W. P. Reinhardt, J. Phys. B **16**, 2103 (1983); H. J. Korsch and R. Möhlenkamp, Z. Phys. A **314**, 267 (1983).
[4] M. Nauenberg, Phys. Rev. Lett. **64**, 2731 (1990); this paper apparently provides the first example of the use of a zero-velocity surface in this problem.
[5] J. A Griffiths and D. Farrelly, Phys. Rev. A **45**, R2678 (1992).
[6] K. Rzazewski and B. Piraux, Phys. Rev. A **47**, R1612 (1993).
[7] D. Farrelly and T. Uzer, Phys. Rev. Lett. **74**, 1720 (1995).
[8] G. W. Hill, Am. J. Math. **1**, 5 (1878).
[9] F. R. Moulton, *An Introduction to Celestial Mechanics*, 2nd ed. (MacMillan, New York, 1914).
[10] V. Szebehely, *Theory of Orbits: The Restricted Problem of Three Bodies* (Academic, New York, 1967).
[11] J. M. A. Danby, *Fundamentals of Celestial Mechanics* (MacMillan, New York, 1962).
[12] R. Greenberg and D. R. Davis, Am. J. Phys. **46**, 1068 (1978).
[13] Howard ''borrows'' the term zero-velocity surface from celestial mechanics (Ref. [1], p. 3936) but, in doing so, one must distinguish carefully between the terms ''potential energy surface'' and ''zero-velocity surface'': all of the effective potentials computed by Howard are obtained by setting the momenta to zero in a Hamiltonian having positive definite kinetic energy since the angular momentum is a conserved quantity. Curves of zero velocity are obtained, instead, by setting the mechanical velocities to zero [10,11]: while a zero-velocity surface *may* be equivalent to a potential energy surface (e.g., when the problem contains no velocity-dependent forces) it is not necessarily true that they *must* be equivalent. A salient example is the Hamiltonian (5.1) in [1]. The zero-velocity surface as a limiting surface for motion was first discussed by Hill almost a century and a quarter ago in relation to the motions of the Moon.
[14] A. Peregrine-Smew, D Farrelly, and T. Uzer, Phys. Rev. A **51**, 4293 (1995).
[15] J. E. Howard, Phys. Rev. A **46**, 364 (1992).
[16] M. A. Murison, Ph.D. thesis, University of Wisconsin, (UMI Dissertation Services, Ann Arbor, MI, 1988).
[17] R. Abraham and J. E. Marsden, *Foundations of Mechanics*, 2nd ed. (Addison-Wesley, Redwood City, CA, 1987).
[18] I. Bialynicki-Birula, M. Kaliński, and J. H. Eberly, Phys. Rev. Lett. **73**, 1777 (1994).
[19] J. E. Howard, Celest. Mech. Dynamical Astron. **48**, 267 (1990).
[20] E. J. Routh, Proc. London Math. Soc. **6**, 86 (1875).
[21] A. Deprit and A. Deprit-Bartolomé, Astron. J. **72**, 173 (1967).
[22] A. Deprit and J. Henrard, Adv. Astron. Astrophys. **6**, 1 (1968).
[23] D. Farrelly, E. Lee, and T. Uzer, Phys. Rev. Lett. **75**, 972 (1995).
[24] I. Bialynicki-Birula, M. Kaliński, and J. H. Eberly, Phys. Rev. Lett. **75**, 973 (1995).
[25] P. S. Epstein, Ann. Phys. (Leipzig) **1**, 489 (1916); K. Schwarzschild, Sitzungsber. Dtsch. Akad. Wiss. Berlin Kl. Math. Phys. Tech., 548 (1916).
[26] D. Farrelly and T. Uzer, Celest. Mech. Dynamical Astron. **61**, 71 (1995).