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Action-angle variables for the diamagnetic Kepler problem

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The diamagnetic Kepler problem, or quadratic Zeeman effect in hydrogen, is converted into an asymmetric top via a transformation to Lissajous action-angle variables. These variables are especially suitable for uniform semiclassical quantization of the system for arbitrary values of the azimuthal quantum number m.

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The connection between the hydrogen atom and the harmonic oscillator is well known and is related to the existence of the Runge-Lenz vector as an extra conserved quantity [1]. When an external field is applied to the system the basic zero-order symmetry is broken, but approximately conserved quantities might persist. In the diamagnetic Kepler problem [quadratic Zeeman effect (QZE)], an approximate constant of motion was found independently by Solov'ev [2] and Herrick [3] (see also Reinhardt and Farrelly [4]). This constant, usually denoted Λ, is given explicitly by

$$\Lambda=4\,\mathbf{A}^2-5\,\mathbf{A}_z^2\ , \tag{1}$$

where

$$\mathbf{A}=\frac{1}{\sqrt{-2H_0}}\left[\mathbf{p}\times\mathbf{L}-\frac{\mathbf{r}}{r}\right] \tag{2}$$

is the modified Runge-Lenz vector and H_0 is the unperturbed energy. If the azimuthal quantum number $m=0$, Λ takes values in the range $(-n^2,4n^2)$, where n is the principal quantum number. Depending upon the sign of Λ the classical motion falls into one of two categories: for negative values of Λ it is vibrational, while if Λ is positive the dynamics is rotational. A separatrix between the two kinds of motion occurs when $\Lambda=0$. Extreme positive values of Λ correspond to the ridge states of Fano [5] and it is this motion, localized in the x-y plane, that gives rise to the famous quasi-Landau spacings [6]. Despite much study an outstanding problem in the theory of the QZE is the semiclassical quantization of Λ. Most of the proposed semiclassical quantization formulas are singular at the separatrix between the two kinds of dynamics. To skirt this problem a variety of piecewise quantization rules has been developed (for reviews see Hasegawa, Robnik, and Wunner [7]), but only recently has a *uniform* semiclassical quantization procedure been developed based on the conversion of the QZE Hamiltonian into a perturbed four-dimensional anisotropic oscillator [8,9]. Alongside attempts to develop semiclassical quantization rules there has also been an effort to understand the underlying symmetry of the QZE [10,11]. Uzer [10] has shown that for the $m=0$ case the problem can be mapped onto an asymmetric top by using classical perturbation theory and the SU(2) symmetry of the harmonic oscillator.

In this Brief Report a canonical transformation to a set of action-angle variables is made that is especially appropriate to the application of uniform semiclassical quantization methods [8,9,12]. This provides an alternative route to, and an independent check of, the more complicated analyses contained in Refs. [8] and [9]. The approach described also has the merit of providing a direct path to the asymmetric top mapping developed by Uzer [10].

In atomic units the QZE Hamiltonian is the following:

$$H=E=\tfrac{1}{2}(P_x^2+P_y^2+P_z^2)-\frac{1}{r}+\frac{1}{8}\gamma^2(x^2+y^2)\ , \tag{3}$$

where γ is the magnetic-field strength and the paramagnetic term has been transformed away [4]. The axial symmetry preserves m as a good quantum number and thus the problem may be reduced to two dimensions. This can be achieved by a transformation to the "squared" parabolic coordinates,

$$x=uv\cos\vartheta,\quad y=uv\sin\vartheta,\quad z=\tfrac{1}{2}(u^2-v^2)\ , \tag{4}$$

which converts the Hamiltonian into the following:

$$H=\frac{1}{2(u^2+v^2)}\left[P_u^2+P_v^2+\frac{m^2}{u^2}+\frac{m^2}{v^2}-4\right]+\tfrac{1}{8}\gamma^2u^2v^2 . \tag{5}$$

Multiplication by (u^2+v^2)—in essence a classical regularization [13]—leads to the Hamiltonian

$$K=2=\frac{1}{2}\left[P_u^2+P_v^2+4\omega^2(u^2+v^2)+\frac{m^2}{u^2}+\frac{m^2}{v^2}\right] \tag{6}$$
$$+\frac{1}{8}\gamma^2(u^2+v^2)(u^2v^2) ,$$

where

$$2\omega^2=-E . \tag{7}$$

Aside from the centrifugal terms, the Hamiltonian resembles two nonlinearly coupled harmonic oscillators. When $m=0$ the QZE reduces to a single two-dimensional harmonic oscillator with a quartic coupling term. This version of the QZE has been widely studied theoretically because of the simple form of the Hamiltonian [4,8–10,14–16]. For nonzero m the centrifugal terms complicate any transformation to action-angle variables and hinder the application of classical perturbation theory. Consequently, for nonzero m most studies using classical perturbation theory have been in terms of the Delaunay elements [17–19]. Unfortunately these variables turn out to be unsuited to uniform semiclassical quantization of motion in the propinquity of the separatrix [7–9]. These problems are avoided by a transformation from the parabolic coordinates and momenta to a new set of action-angle variables (Deprit's "Lissajous" elements) (Φ,ϕ) and (Ψ,ψ) [18,19]. This is accomplished by means of the generating function $W=W_1(u,\Phi)+W_2(v,\Psi)$, which is of the F_2 type. W satisfies

$$P_u=\frac{\partial W}{\partial u},\quad \phi=\frac{\partial W}{\partial \Phi},\quad P_v=\frac{\partial W}{\partial v},\quad \psi=\frac{\partial W}{\partial \Psi} . \tag{8}$$

The generating function $W_1(u,\Phi)$ is obtained from the Hamilton-Jacobi equation

$$\frac{1}{2}\left[\frac{\partial W_1}{\partial u}\right]^2+\frac{m^2}{2u^2}+2\omega^2u^2=2\omega\Phi , \tag{9}$$

with a similar equation for $W_2(v,\Psi)$. Solving for $W_1(u,\Phi)$ gives

$$W_1(u,\Phi)=\int_{u_1}^{u}du\left[4\omega\Phi-4\omega^2u^2-\frac{m^2}{u^2}\right]^{1/2} , \tag{10}$$

where u_1 is the positive root of the radicand [and similarly for $W_2(v,\Psi)$]. Defining the quantities

$$\alpha(\Phi,m)=\frac{(\Phi^2-m^2)^{1/2}}{\Phi},\quad \beta(\Psi,m)=\frac{(\Psi^2-m^2)^{1/2}}{\Psi} , \tag{11}$$

and using Eq. (7) gives

$$u^2=\frac{\Phi}{2\omega}[1-\alpha\cos(2\phi)],\quad v^2=\frac{\Psi}{2\omega}[1-\beta\cos(2\psi)] , \tag{12}$$

which allows the Hamiltonian K to be written in the form

$$K=2=2\omega(\Phi+\Psi)+\tfrac{1}{8}\gamma^2H_1(m;\Phi,\phi,\Psi,\psi) . \tag{13}$$

The functional form of H_1 will not be given here but is readily obtained by direct substitution of Eq. (12) into Eq. (6). At this point all of the transformations are exact and Eq. (13) represents the QZE Hamiltonian in terms of harmonic-oscillator-like action-angle variables. Averaging the perturbation in these variables is straightforward and avoids the use of involved classical perturbation methods like Birkhoff-Gustavson normal form theory [4,8–10,20,21]. More importantly it leads to a Hamiltonian expressed in terms of a set of actions especially useful for quantization. Contemplation of Eq. (7) reveals that not all of the states of the oscillator match up with QZE states [8,9]. Those that do satisfy,

$$\Phi+\Psi=2n . \tag{14}$$

In light of this a further canonical transformation is introduced,

$$\Phi=n+j_z,\quad \phi=\tfrac{1}{2}(\phi_n+\phi_z) , \tag{15}$$

$$\Psi=n-j_z,\quad \psi=\tfrac{1}{2}(\phi_n-\phi_z) , \tag{16}$$

where ϕ_n is the angle conjugate to the principal Kepler action n. This is the angle to be averaged over. Doing so [22] gives the following expression for H_1:

$$H_1=\frac{n}{8\omega^3}(\Lambda+m^2+n^2) , \tag{17}$$

where the term in Λ has been singled out for convenient comparison with the results of Robnik and Schrüfer [20] and Kuwata, Harada, and Hasegawa [21]. In terms of the new action-angle variables,

$$\Lambda=2\{[(n+j_z)^2-m^2][(n-j_z)^2-m^2]\}^{1/2}\cos2\phi_z$$
$$-3j_x^2-2m^2+2n^2 \tag{18}$$

with $|j_z|\le|(n-|m|)|$. This expression agrees to this order of perturbation theory with that obtained in Refs. [8] and [9]. Level curves of $\Lambda(m;j_z,\phi)$ resemble those of a twofold hindered rotor when $m=0$. In the rotor picture the *localized* vibrational states of the QZE correspond to the *localized* rotational states of the rotor, which approximately conserve j_z. Analysis of Eq. (18) reveals that as m is progressively increased, the vibrational states start to disappear until at the point where $m/n=1/\sqrt{5}$ they have vanished altogether [17,18] and Λ takes only positive values.

The problem can also be mapped onto a generalized angular momentum $\mathbf{J}(J_x,J_y,J_z)$ by means of the following transformation [23]:

$$J_z=j_z/2,\quad \theta_z=2\phi_z . \tag{19}$$

In terms of the new variables the other components of $\mathbf{J}$ are defined as follows:

$$J_x=(J^2-J_z^2)^{1/2}\sin\theta_z, \quad J_y=(J^2-J_z^2)^{1/2}\cos\theta_z \ , \tag{20}$$

with

$$J^2=|\mathbf{J}|^2=\frac{(n-|m|)^2}{4} \ . \tag{21}$$

In the limit $m=0$ the problem is thus equivalent to an asymmetric top, as discussed by Uzer [10].

In conclusion, Eq. (18) is in an especially tractable form for the application of uniform semiclassical quantization procedures using hindered-rotor-like quantization formulas [24,25] because the action j_z is uniformly valid through the separatrix.

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