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Dynamical symmetry of the quadratic Zeeman effect in hydrogen: Semiclassical quantization

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By exploiting the approximate SU(2) symmetry of the $m=0$ quadratic Zeeman Hamiltonian within multiplets of fixed principal quantum number, the dynamics is mapped onto a twofold hindered rotor. This allows a singularity-free uniform semiclassical quantization of Solov'ev's approximate integral of the motion to be performed. Excellent agreement with quantum results is obtained.

The proposal by Zimmerman, Kash, and Kleppner[1] in 1980 that the hydrogen atom in a strong magnetic field [the quadratic Zeeman effect (QZE)] possesses a hidden symmetry marked the start of a decade of extraordinary theoretical and experimental interest in this problem.[2,3] Nevertheless, the quadratic Zeeman effect (QZE) continues to be one of the most challenging unsolved problems in atomic physics and nonlinear dynamics. In the opposite limits of very weak and very strong magnetic fields the Hamiltonian is almost integrable, whereas in the regime where the Coulomb and magnetic fields are comparable the dynamics is strongly chaotic. The accessibility of the QZE to both experimental and theoretical studies makes it an ideal system on which to probe issues relating to chaos and the correspondence principle. With this in mind, semiclassical methods have featured prominently in studies of the QZE, proving invaluable, for example, in explaining the different series of quasi-Landau resonances observed in photoabsorption spectra.[4–6] Despite successes, however, the semiclassical theory of the QZE remains primitive; the most apparent and long-standing problem being the lack of a canonically invariant, singularity-free quantization formula covering the topologically distinct kinds of trajectories which can arise.[3]

Through second order in the magnetic field, the "hidden" dynamical constant of motion was shown by Solov'ev[7] to be

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

where $\mathbf{A}$ is essentially the Runge-Lenz vector,

$$\mathbf{A} = (\mathbf{p}\times\mathbf{L} - \mathbf{r}/r)/(-2mH)^{1/2}\,, \tag{2}$$

and Λ lies in the range $-1 \le \Lambda \le 4$. The two extremal values correspond to different limiting types of classical motion, usually labeled rotational $(\Lambda > 0)$ and vibrational $(\Lambda < 0)$, with the separatrix occurring at $\Lambda = 0$.[3,8] Solov'ev's invariant (Λ) is a consequence of the approximate separability of the QZE through second order in the magnetic field in elliptical cylindrical coordinates on the O(4) sphere.[9–11] The quantum evaluation of Λ is fairly straightforward involving the simultaneous diagonalization of the zero-order Hamiltonian, L_z and Λ, after which low-order perturbation theory can be used to estimate the QZE energies.[12,13] In contrast, semiclassical methods have the potential advantage of providing the means of generating and quantizing much higher-order approximations to the hidden constant of the motion than Λ.

There have been several attempts,[3,5,8,14–16] starting with Solov'ev,[7] to quantize Λ semiclassically, but all have encountered difficulties due to singularities in the quantization formulas occurring at the separatrix between rotational and vibrational types of classical motion, and none has been able to incorporate tunneling in any consistent way. The object of this Rapid Communication is to resolve difficulties associated with the semiclassical quantization of Λ, which is of considerable experimental and theoretical importance.[8] Classical perturbation theory is first used to normalize the QZE after which a canonically invariant uniform semiclassical quantization formula is obtained for Λ in terms of action-angle variables based on the SU(2) symmetry of the system.

In cylindrical coordinates and atomic units $(m=e=\hbar=1)$ the QZE is two dimensional, with the Hamiltonian given by

$$H = E = \tfrac{1}{2}(P_\rho^2 + P_z^2) + \frac{P_\phi^2}{2\rho^2} + \frac{1}{8}\gamma^2\rho^2 - \frac{1}{(\rho^2+z^2)^{1/2}}\,, \tag{3}$$

where E is the energy,

$$\rho^2 = x^2 + y^2\,,$$

and the reduced field, $\gamma = B/(2.35\times 10^5\ \mathrm{T})$. The discussion is simplified by considering only the $m=0$ $(P_\phi = m\hbar = 0)$ case which has been the subject of most experimental studies[2–6] and is quite representative of the dynamics for all m. Classically, the $m=0$ case displays numerical pathologies because trajectories can penetrate the Coulomb singularity at the origin. This problem can be avoided by transforming to "regularized" parabolic coordinates[15] which also make the SU(2) symmetry of the system apparent, and facilitate application of classical perturbation theory. Upon setting $\rho = uv$, $z = (u^2 - v^2)/2$, making a time transformation, and performing a trivial canonical transformation to normalize the oscillator frequencies, the $m=0$ Hamiltonian becomes

$$\mathcal{H} = \frac{1}{(-2E)^{1/2}} = \tfrac{1}{2}(p_u^2 + u^2) + \tfrac{1}{2}(p_v^2 + v^2) + \frac{\gamma^2}{32E^2}(u^2+v^2)u^2v^2\,. \tag{4}$$

The SU(2) algebra is generated by the following quantities:

$$\pi_1 = \tfrac{1}{2}(p_u^2+u^2) - \tfrac{1}{2}(p_v^2+v^2)\,, \tag{5a}$$

$$\pi_2 = vp_u - up_v\,, \tag{5b}$$

$$\pi_3 = p_u p_v + uv\,, \tag{5c}$$

which commute with the zero-order energy,

$$\pi_0 = \mathcal{H}_0 = \tfrac{1}{2}(p_u^2+u^2) + \tfrac{1}{2}(p_v^2+v^2) \tag{5d}$$

and satisfy the Poisson bracket relations,

$$\{\pi_j,\pi_k\} = \epsilon_{jkl}\pi_l \tag{6a}$$

together with the relation,

$$\pi_0^2 = \pi_1^2+\pi_2^2+\pi_3^2\,. \tag{6b}$$

Using classical (Birkhoff-Gustavson) perturbation theory an integrable approximation (the *normal form* denoted $\mathcal{H}_{\rm NF}$) to $\mathcal{H}$ can be found as a power series in coordinates and momenta. The normal form was originally obtained in Ref. 15, which was an independent determination of Solov'ev's invariant for $m=0$ to high order in the field.[3,10,14] In terms of the SU(2) generators the normal form to order γ^2 is[14]

$$\mathcal{H}_{\rm NF} = \pi_0 + c\pi_0[5(\pi_0^2-\pi_1^2) - 4\pi_2^2]\,, \tag{7}$$

where $c=\gamma^2/256E^2$. Using group-theoretical methods it is possible to show that the approximate constant of motion obtained from the normal form is equivalent to Λ.[17] In particular, π_1 can be identified with A_z and π_2^2 with $\mathbf{A}^2$ to within constants. Semiclassical quantization of Eq. (7) is complicated by the zero-order resonance in Eq. (4) making the transformation to action-angle variables nontrivial. This problem can be solved using a general Lie algebraic approach to the uniform semiclassical quantization of resonant systems developed previously.[18] One choice of actions is the following, where Eqs. (4) and (5d) have been used to quantize J_1,

$$\begin{aligned} \pi_0 &= J_1 = 2n\,,\\ \pi_1 &= J_2\,,\\ \pi_2 &= \sqrt{J_1^2-J_2^2}\cos 2\phi_2\,,\\ \pi_3 &= \sqrt{J_1^2-J_2^2}\sin 2\phi_2\,, \end{aligned} \tag{8}$$

with ϕ_2 in the range $0\le\phi_2\le\pi$. Although this is not the only choice possible [in general the spherical symmetry allows the subscripts between π_1, π_2, and π_3 in Eq. (8) to be interchanged in any order, see Eq. (6b)] it turns out to be the best choice of J_2 consistent with the actual dynamics of the QZE. This is because the generator π_1 is proportional to A_z, which is almost a good constant of motion for the localized vibrational states (for these states $\Lambda \sim -A_z^2$).

Because J_1 is conserved, quantization of J_2 may be performed in terms of the auxilliary quantity [see Eq. (7)],

$$\mathcal{E} = 5(\pi_0^2-\pi_1^2) - 4\pi_2^2\,, \tag{9}$$

the form of which is particularly suggestive when compared to Eq. (1). Transforming the Runge-Lenz vector into regularized coordinates gives $\Lambda = \mathcal{E}/J_1^2 - 1$, where $\mathcal{E}$ is restricted to the range $0\le\mathcal{E}\le 5J_1^2$ since $0\le J_2\le J_1$. Combining Eqs. (8) and (9) and solving for the action J_2 gives

$$J_2 = \left[J_1^2 - \frac{\mathcal{E}}{5-4\cos^2 2\phi_2} \right]^{1/2}. \tag{10}$$

The phase portrait of J_2 as a function of ϕ_2 is shown in Fig. 1 and is a twofold hindered rotor. At this point it should be noted that because the transformation from cylindrical to regularized coordinates is nonlinear, doubling the size of phase space, only half of the states of the oscillator match up with actual states of the QZE; these are those *oscillator* states of even-even parity.[14] The states in the wells correspond to *rotational* ($\Lambda>0$) states of the original Hamiltonian (3) while the vibrational states ($\Lambda<0$) of Eq. (3) have been mapped onto rotational states in the rotor picture. This might seem puzzling: However, the original vibrational trajectories are *localized* in two disjoint regions of phase space when the dynamical constant Λ is negative,[13] and the transformation to regularized coordinates maps these trajectories into *local* mode states of the oscillator. Since local modes in the oscillator picture are those maximizing (and conserving) $|\pi_1|$, they correspond to the rotational states of the rotor, which do (almost) conserve J_2 as they should.[17,19] This is why π_1 was chosen as the generator to be quantized; other choices are either singular at the separatrix ($J_2=\pi_2$) or give poorer agreement with quantum results ($J_2=\pi_3$), not being appropriate to the topology of the trajectories. The oscillator *normal* mode states[13] in the wells ($\Lambda>0$) become the ridge states of Fano[20] as Λ approaches its maximum value. The stability of these states against "falling" off the ridge can now be understood since they exist at the bottom of a well in action-angle space. In the harmonic-oscillator picture these states behave like asymmetric normal modes, being essen-

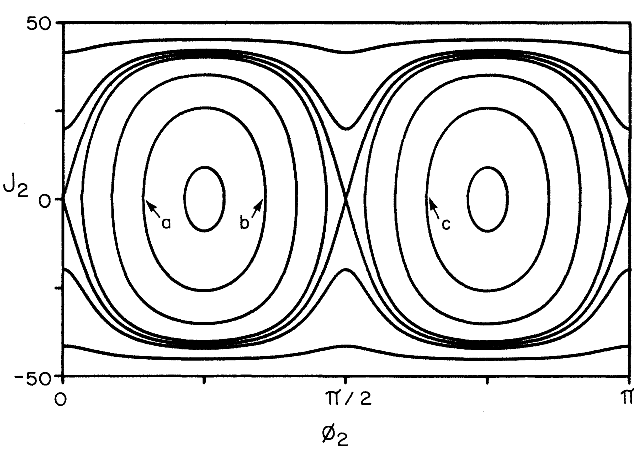

FIG. 1. Phase plot of J_2 at various values of Λ between its minimum and maximum values, as determined using Eq. (10) with $J_1=2n=46$. The rotorlike states correspond to $\Lambda<0$ while the states in the wells have $\Lambda>0$. The classical turning points a, b, and c used in the evaluation of the phase integrals are illustrated at an arbitrary value of Λ.

tially localized in one well or the other.

The uniform semiclassical quantization formula for the twofold hindered rotor which accounts for tunneling is[21,22]

$$\alpha-\Phi(\epsilon)=k\pi\pm\tan^{-1}(e^{-\pi\epsilon}),\quad k=1,2,\ldots,2\,\mathrm{int}(n/2), \tag{11}$$

where int takes the integer part of its argument. The phase integrals are given by

$$\begin{aligned}\alpha&=\int_a^b J_2 d\phi_2 \text{ for vibrators},\\ \alpha&=\int_0^{\pi/2} J_2 d\phi_2 \text{ for rotators},\\ \pi\epsilon&=-\int_b^c |J_2| d\phi_2,\end{aligned} \tag{12}$$

and the classical turning points, a, b, and c (shown in Fig. 1) are complex for states above the barrier tops. The quantum correction function Φ is an antisymmetric function of its argument and is defined by[22]

$$\Phi(\epsilon)=\epsilon+\arg[\Gamma(\tfrac{1}{2}+i\epsilon)]-\epsilon\ln|\epsilon|. \tag{13}$$

Every k gives rise to two states ($\pm$), but only half of these states correspond to states of the QZE. The subseparatrix normal-mode states occur in pairs but only one member of a pair can map back into each rotational state in the original cylindrical coordinates (the Zeeman rotational states are not split by tunneling). Below the separatrix only the symmetric states of the rotor qualify and these are obtained by taking the minus sign in Eq. (11) corresponding to the a_{k-1} state in Mathieu notation.[21,22] Above the barrier the required states have k *even* (in a primitive quantization of these levels, $\alpha = k\pi$, with k even) and the degeneracy between the $\pm$ states is lifted due to tunneling between the vibrational Zeeman states. Most importantly the quantization formula is completely singularity free and passes uniformly through the separatrix separating vibrational from rotational states. Results obtained from the semiclassical quantization condition are presented in Table I and are clearly in excellent agreement with quantum results. Interestingly the doublets in the quantized values of Λ are *not* due to tunneling through the rotor barrier in this picture. The splittings are a consequence of dynamical tunneling and occur as a result of reflection above the barrier tops.

TABLE I. Quantum (Refs. 12 and 13) (Λ^{qm}) and semiclassical (Λ^{sc}) values of Solov'ev's invariant for the $n=23$ ($m=0$) manifold; $k^{\pm}$ refers to Eq. (11). The separatrix occurs classically when $\Lambda=0$.

$k^{\pm}$	Λ^{qm}	Λ^{sc}	$k^{\pm}$	Λ^{qm}	Λ^{sc}
22^+	−0.815 18	−0.811 77	12^-	0.659 82	0.662 49
22^-	−0.815 18	−0.811 77	11^-	0.858 67	0.861 21
20^+	−0.474 47	−0.471 03	10^-	1.075 54	1.077 86
20^-	−0.474 45	−0.471 01	9^-	1.309 82	1.312 16
18^+	−0.191 24	−0.187 67	8^-	1.561 67	1.563 92
18^-	−0.188 60	−0.185 09	7^-	1.830 84	1.833 02
16^+	−0.006 50	−0.002 71	6^-	2.117 24	2.119 36
	Separatrix		5^-	2.420 82	2.422 87
16^-	0.050 73	0.054 13	4^-	2.741 15	2.743 50
15^-	0.179 02	0.178 97	3^-	3.079 30	3.081 22
14^-	0.317 83	0.320 83	2^-	3.434 14	3.435 99
13^-	0.479 35	0.482 14	1^-	3.806 02	3.807 78

This analysis has provided a singularity-free, uniform, semiclassical quantization of the QZE. It should be noted that Robnik and Schrüfer's quantization involved diagonalization of the normal form in a quantum-mechanical basis and was therefore not a canonically invariant semiclassical approximation.[14] The semiclassical method also has the advantage that ordering of operators is not an issue. The Lie algebraic picture developed here is crucial to constructing a scheme by which to quantize the QZE to higher order in the field and/or for $m\neq 0$.

Note added in proof. Since this paper was submitted a paper by Uzer[23] has appeared in which the QZE is mapped onto an asymmetric top, providing a complementary view to that of this paper.

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