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LETTER TO THE EDITOR

## The Bohr-Sommerfeld quantisation for a ring-shaped potential

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**Abstract.** Using the Bohr-Sommerfeld quantisation rule, we obtain the correct energy spectrum of the Hartmann potential. We also analyse the degeneracies found for this problem in the classical context.

In a recent paper published in this journal [1], Kibler and Winternitz discussed the dynamical invariance algebra associated with the Hartmann potential [2]. It belongs to a class of ring-shaped potentials that show, like the Coulomb does, an extra degeneracy. These are examples of potentials that exhibit an 'accidental degeneracy'—a degeneracy not explained in a simple way by the existence of a geometric symmetry.

The Hartmann potential was introduced in 1972 [2] to account for some axial symmetric systems in quantum chemistry, such as some ring-shaped molecules. Since then, it has been solved using many different approaches either classically [1] or quantum mechanically [1, 3-6].

In this letter we first show that the straightforward application of the Bohr-Sommerfeld quantisation rule [7], based on the action-angle variables, leads to the correct spectrum for the bound states associated with the Hartmann potential. In the second place, we also use the action-angle variables to analyse classically the origin of the degeneracy found for the energy levels.

We begin by making a brief review of the classical formalism to be used later. For more details the reader may consult [7]. Let us consider a classical system with  $n$  degrees of freedom described by the Hamiltonian  $H(q_1, \dots, q_n, p_1, \dots, p_n)$ . The Hamilton-Jacobi (HJ) equation is given by

$$H\left(q_i, p_i = \frac{\partial S}{\partial q_i}\right) + \frac{\partial S}{\partial t}(q_i, P_i, t) = 0 \quad (1)$$

where the classical action  $S$  is identified with the generating function of a canonical transformation which leads to the new set of canonical variables  $\{Q_i, P_i\}$ . The HJ equation is nothing more than the statement that the new Hamiltonian is identically zero.

If the Hamiltonian is time independent we can write

$$S(q_i, P_i, t) = W(q_i, P_i) - Et \quad (2)$$

where  $W(q_i, P_i)$  is called the Hamilton principal function. Using equation (2) the HJ equation takes the form

$$H\left(q_i, P_i = \frac{\partial W}{\partial q_i}\right) = E. \quad (3)$$

If a physical system describes a periodic motion, either a rotation or a libration, we can make a canonical transformation into a new set of canonical variables, called action-angle variables, which are extremely convenient for dealing with such systems. In particular, using these variables we can obtain the frequencies of the system without even solving the problem at hand.

The action variables are defined as

$$J_i \equiv \oint P_i dq_i \quad i = 1, 2, \dots, n \quad (4)$$

while the angle variables are given by

$$\omega_i = \frac{\partial W(q_i, J_i)}{\partial J_i} \quad i = 1, 2, \dots, n \quad (5)$$

where, as usual, we write the Hamilton function in terms of the constants of motion  $J_i$ . Hamilton's equations take the form

$$\dot{J}_i = \frac{\partial H}{\partial \omega_i}(J_1, \dots, J_n) = 0 \quad (6a)$$

$$\dot{\omega}_i = \frac{\partial H}{\partial J_i}(J_1, \dots, J_n) \equiv \nu_i(J_1, \dots, J_n). \quad (6b)$$

From (6a) we see that the  $J_i$  are actually constants. Since the  $\nu_i$  are given only in terms of these constants, they are also constants and the direct integration of (6b) yields

$$\omega_i = \nu_i t + \beta_i \quad i = 1, 2, \dots, n. \quad (7)$$

It can be shown that the  $\nu_i$  in the above equations are the frequencies associated with the periodic motion of the  $q_i$  [7]. Hence, in order to get these frequencies there is no need to solve the problem at all. We just define the  $J_i$ , write the Hamiltonian as  $H(J_1, \dots, J_n)$  and then evaluate  $\nu_i = \partial H / \partial J_i$ .

When there are  $m$  relations among the frequencies, written as

$$\sum_{i=1}^n b_{ik} \nu_i = 0 \quad k = 1, 2, \dots, m \quad (8)$$

where the  $b_{ik}$  are rational numbers, we say that the system is  $m$ -degenerated. When  $m = n - 1$  we say that the system is completely degenerated, as for example the Kepler problem. In this case, all frequencies are commensurable—which means that any  $\nu_i$  may be expressed as a rational number times any other  $\nu_j$ —and the motion is periodic or, in other words, the particle describes a closed trajectory.

Suppose now we are dealing with an  $m$ -degenerated system. Since not all the frequencies are independent of each other (there are only  $n - m$  independent ones), we can eliminate the redundant frequencies. This is achieved by a suitable point canonical transformation from the original set of variables  $\{J_i, \omega_i\}$  to a new set of action-angle variables  $\{J'_i, \omega'_i\}$  for which  $m$  of the associated frequencies  $\nu'_j$  vanish. It is easy to show that the generating function for this transformation is given by

$$F_2(\omega_i, J'_i) = \sum_{k=1}^m \sum_{i=1}^n J'_k b_{ik} \omega_i + \sum_{k=m+1}^n J'_k \omega_k \quad (9)$$

with the same  $b_{ik}$  appearing in (8).

Observing, then, that  $F_2(\omega_i, J'_i)$  is a generating function of the second kind, we have

$$\omega'_k = \frac{\partial F_2}{\partial J'_k} = \begin{cases} \sum_{i=1}^m b_{ik} \omega_i & \text{if } k = 1, 2, \dots, m \\ \omega_k & \text{if } k = m+1, \dots, n. \end{cases} \quad (10)$$

Differentiating equation (10) and using equation (6b), we obtain

$$\nu'_k = \sum_{i=1}^n b_{ik} \nu_i = 0 \quad \text{for } k = 1, 2, \dots, m \quad (11a)$$

$$\nu'_k = \nu_k. \quad (11b)$$

Looking at equation (6b) we can also conclude that the Hamiltonian must be independent of the action variables  $J'_i$  for which the associated frequencies  $\nu'_i$  vanish. Hence, for an  $m$ -degenerated system the Hamiltonian can always be written in terms of only  $n - m$  action variables. Following Sommerfeld we will call them 'proper action variables'. We can obtain the  $J'_i$  through an inversion of the  $n$  transformation equations

$$J'_i = \frac{\partial F_2}{\partial \omega_i} = \sum_{k=1}^m J'_k b_{ki} + \sum_{k=m+1}^n J'_k \delta_{ki}. \quad (12)$$

The Bohr-Sommerfeld quantisation rule is implemented by the following substitution:

$$J'_i \Rightarrow nh \quad (13)$$

where  $n$  is a positive integer number and  $h$  is the Planck constant.

As a final comment before applying this formula to the Hartman potential, let us observe that, in general, the degeneracies become clear when we write the Hamiltonian in terms of the action variables and its functional dependence is analysed with these variables. Let us now apply the Bohr-Sommerfeld quantisation rule to obtain the energy spectrum for the Hartmann potential. Using spherical coordinates it can be written as

$$V(r, \theta) = -\frac{\alpha}{r} + \frac{\beta}{r^2 \sin^2 \theta} \quad (14)$$

where we defined

$$\alpha \equiv -2\eta\sigma^2 a_0 \varepsilon_0 \quad (15a)$$

$$\beta \equiv -\eta^2 \sigma^2 a_0^2 \varepsilon_0 q. \quad (15b)$$

In the above equations,  $a_0$  is the Bohr radius,  $\varepsilon_0$  the energy for the ground state of the hydrogen atom,  $\eta$  and  $\sigma$  are positive parameters whose variation allows different applications in quantum chemistry and  $q$  was introduced in order to regain the Coulomb potential for the particular case  $q = 0$ .

However, it is convenient to work with parabolic coordinates  $(a, b, \phi)$ , defined as [8]

$$x = \sqrt{ab} \cos \phi \quad (16a)$$

$$y = \sqrt{ab} \sin \phi \quad (16b)$$

$$z = \frac{1}{2}(a - b). \quad (16c)$$

The Hartman potential written in terms of these variables takes the form

$$V(a, b, \phi) = -\frac{2\alpha}{a+b} + \frac{\beta}{ab}. \quad (17)$$

The classical Lagrangian is then given by

$$\mathcal{L} = \frac{m}{2} \left\{ \frac{\dot{a}^2}{4} + \frac{b\dot{a}^2}{4a} + \frac{a\dot{b}^2}{4b} + \frac{\dot{b}^2}{4} + ab\dot{\phi}^2 \right\} - \frac{2\alpha}{a+b} + \frac{\beta}{ab}. \quad (18)$$

Making the Legendre transformation we get the Hamiltonian

$$\begin{aligned} H(p_a, p_b, p_\phi; a, b) &= p_a \dot{a} + p_b \dot{b} + p_\phi \dot{\phi} - \mathcal{L} \\ &= \frac{2}{m} \left\{ \frac{a}{a+b} p_a^2 + \frac{b}{a+b} p_b^2 + \frac{p_\phi^2}{4ab} \right\} - \frac{2\alpha}{a+b} + \frac{\beta}{ab} \end{aligned} \quad (19)$$

where  $p_a$ ,  $p_b$  and  $p_\phi$  are the canonical momenta conjugated to the variables  $a$ ,  $b$  and  $\phi$  respectively. As is well known, the HJ equation is completely separable in these coordinates (as well as in spherical ones). This means that we can write

$$S = W - Et = W_a(a) + W_b(b) + W_\phi(\phi) - Et. \quad (20)$$

From equations (20), (19) and (3) we have

$$\left[ \frac{4a^2b}{a+b} \left( \frac{\partial W_a}{\partial a} \right)^2 + \frac{4b^2a}{a+b} \left( \frac{\partial W_b}{\partial b} \right)^2 + \left( \frac{\partial W_\phi}{\partial \phi} \right)^2 \right] - \frac{4mab^\alpha}{a+b} + 2m\beta = 2mabE \quad (21)$$

where we have multiplied the whole expression by  $2mab$ . As usual, we set

$$\left( \frac{\partial W_\phi}{\partial \phi} \right)^2 = \alpha_\phi^2 \quad (22)$$

whose solution is obvious. However, we do not need to solve the equations for  $W_\phi$ ,  $W_a$  and  $W_b$ , since we are not interested in the solution of the problem. Essentially, all we need in order to proceed with the Bohr-Sommerfeld quantisation is to obtain explicitly all the action variables and then write the Hamiltonian in terms of them. For  $J_\phi$  we readily obtain

$$J_\phi = \oint \frac{\partial W_\phi}{\partial \phi} d\phi = 2\pi\alpha_\phi. \quad (23)$$

Multiplying equation (21) by  $(a+b)/ab$  and making use of the identity

$$\frac{a+b}{ab} = \frac{1}{a} + \frac{1}{b}$$

we get

$$4a \left( \frac{\partial W_a}{\partial a} \right)^2 + 4b \left( \frac{\partial W_b}{\partial b} \right)^2 + 2m\beta \left( \frac{1}{a} + \frac{1}{b} \right) - 4m\alpha - 2mE(a+b) = -\alpha_\phi^2 \left( \frac{1}{a} + \frac{1}{b} \right) \quad (24)$$

where we used  $J_\phi = 2\pi\alpha_\phi$ . Separating variables in the above equation and using the definition of the action variables, we have

$$J_a \equiv \oint \frac{\partial W_a}{\partial a} da = \oint \left[ \frac{mE}{2} + \frac{\gamma}{4a} - \left( \frac{\alpha_\phi^2 + 2m\beta}{4a^2} \right) \right]^{1/2} da \quad (25a)$$

$$J_b \equiv \oint \frac{\partial W_b}{\partial b} db = \oint \left[ \frac{mE}{2} - \frac{\gamma}{4b} - \left( \frac{\alpha_\phi^2 + 2m\beta}{4b^2} \right) \right]^{1/2} db \quad (25b)$$

where the separation constant  $\gamma$  was chosen as

$$4a \left( \frac{\partial W_a}{\partial a} \right)^2 + \frac{2m\beta}{a} - 2mEa + \frac{\alpha_\phi^2}{b} = \gamma = - \left[ 4b \left( \frac{\partial W_b}{\partial b} \right)^2 + \frac{2m\beta}{b} - 2mEb + \frac{\alpha_\phi^2}{b} \right]. \quad (26)$$

Consulting standard tables [9], we obtain after some rearrangement

$$J_a = -\pi \left( \frac{J_\phi^2}{4\pi^2} + 2m\beta \right)^{1/2} + \left( \frac{2}{m(-E)} \right)^{1/2} \pi \frac{\gamma}{4} \quad (27a)$$

$$J_b = -\pi \left( \frac{J_\phi^2}{4\pi^2} + 2m\beta \right)^{1/2} + \left( m\alpha - \frac{\gamma}{4} \right) \pi \left( \frac{2}{m(-E)} \right)^{1/2}. \quad (27b)$$

From (27a) we can write  $\gamma$  in terms of  $J_a$

$$\gamma = \left[ J_a + \pi \left( \frac{J_\phi^2}{4\pi^2} + 2m\beta \right)^{1/2} \right] \frac{4}{\pi} \left( \frac{m(-E)}{2} \right)^{1/2}. \quad (28)$$

Now, eliminating  $\gamma$  from (27b) with the aid of (28) we get

$$J_a + J_b = -2\pi \left( \frac{J_\phi^2}{4\pi^2} + 2m\beta \right)^{1/2} + m\alpha\pi \left( \frac{2}{m(-E)} \right)^{1/2}. \quad (29)$$

Finally, we can invert the last equation to write the energy (the Hamiltonian), in terms of the  $J_i$  as

$$H(J_a, J_b, J_\phi) = - \frac{-2m\alpha^2\pi^2}{(J_a + J_b + \sqrt{J_\phi^2 + 8\pi^2 m\beta})^2}. \quad (30)$$

In order to apply the Bohr-Sommerfeld quantisation rule, let us analyse classically the degeneracies of the problem. From equation (30) we readily see that  $\nu_a = \nu_b$ , since  $\partial H / \partial J_a = \partial H / \partial J_b$ . This means that we will be able to express the Hamiltonian in terms of only two action variables. Consequently, one of the associated frequencies will vanish. With this purpose, let us make the canonical transformation to a new set of action-angle variables  $\{\omega_1, \omega_2, \omega_3, J_1, J_2, J_3\}$ , characterised by the generating function

$$F_2(\omega_a, \omega_b, \omega_\phi, J_1, J_2, J_3) = (\omega_a - \omega_b)J_1 + \omega_b J_2 + \omega_\phi J_3. \quad (31)$$

Hence, the following transformation equations give us the relations between the new and the old sets of action variables

$$J_a = \frac{\partial F_2}{\partial \omega_a} = J_1 \quad (32a)$$

$$J_b = \frac{\partial F_2}{\partial \omega_b} = J_2 - J_1 \quad (32b)$$

$$J_\phi = \frac{\partial F_2}{\partial \omega_\phi} = J_3. \quad (32c)$$

Adding equations (32a) and (32b) we get

$$J_a + J_b = J_2. \quad (33)$$

The new angle variables are obtained by

$$\omega_1 = \frac{\partial F_2}{\partial J_1} = \omega_a - \omega_b \quad \omega_2 = \frac{\partial F_2}{\partial J_2} = \omega_b \quad \omega_3 = \frac{\partial F_2}{\partial J_3} = \omega_\phi \quad (34)$$

and then the associated frequencies are given by

$$\nu_1 = \nu_a - \nu_b = 0 \quad \nu_2 = \nu_b \quad \nu_3 = \nu_\phi. \quad (35)$$

The proper action variables are therefore  $J_2$  and  $J_3$ , since the associated frequencies do not vanish. Writing the energy in terms of these variables we have

$$E = \frac{-2m\alpha^2\pi^2}{(J_2 + \sqrt{J_a^2 + 8\pi^2 m\beta})^2}. \quad (36)$$

Proceeding now with the Bohr-Sommerfeld prescription we put

$$J_2 = nh \quad J_3 = ph \quad n, p = 1, 2, \dots \quad (37)$$

and finally obtain the quantum energy spectrum for the bound states of the Hartmann potential

$$E_{np} = \frac{-2m\alpha^2\pi^2}{(nh + \sqrt{p^2 h^2 + 8\pi m\beta})^2} \quad (38)$$

in complete agreement with previous results [1, 3-6]. The particular case of the Coulomb potential can be treated correctly if we put  $\beta = 0$  in (36). However, we see that there still remains a degeneracy ( $J_2$  and  $J_3$  are no longer proper action variables for the problem), since  $\nu_2 = \partial H / \partial J_2 = \partial H / \partial J_3 = \nu_3$ . Therefore, we will be able to define a new set of action variables such that  $J_2 + J_3 = J'_1$  and write

$$E = -\frac{zE_0}{J_1'^2}. \quad (39)$$

Substituting  $J'_1 = nh$  in (39) we obtain the correct energy levels for the hydrogen atom [10].

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