Approximate motion integral for a hydrogen atom in a magnetic field

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It is shown that the Schrödinger equation for highly excited states of a hydrogen atom in a magnetic field **H** allows a separation of variables (within an accuracy of H^4) in elliptical-cylindrical coordinates on a sphere in a four-dimensional momentum space. A new classification and approximate selection rules are proposed for these states.

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A large number of papers have been devoted to the study of the hydrogen atom in a magnetic field. An interest in this area has increased recently as a result of observation of an exponential decrease in the splitting of the energy levels at the quasi-intersection point with an increase in the principal quantum number n.[1,2] To explain this effect, it was argued in Refs. 1 and 2 that an approximate latent symmetry

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exists. In the present paper such a symmetry is found by means of a quasiclassical perturbation theory of the magnetic field. The quasiclassical approximation in this case is justified, since we are dealing with large values of n. The applicability of perturbation theory in the quasi-intersection region was discussed in Ref. 1.

In the unperturbed problem the electron motion occurs along the Keplerian elliptical trajectories. A nontrivial part of the perturbation is the diamagnetic interaction $V=1/2\ \omega^2\rho^2$ (the magnetic field $\mathbf{H}$ is directed along the z axis, $\rho^2=x^2+y^2$, $\omega=2H/c$, $h=m=e=1$, and c is the velocity of light). To calculate the change of the Keplerian trajectory due to the action of a magnetic field, we have used the secular-perturbation method,[3] in which the electron motion is divided into the motion along an unperturbed elliptical trajectory and a slow variation of the ellipse parameters due to perturbation V. We choose the angular momentum $\mathbf{L}=[\mathbf{r}\times\mathbf{p}]$ and the Runge-Lenz vector $\mathbf{A}=[\mathbf{p}\times\mathbf{L}]-\mathbf{r}/r$ as the parameters that specify the ellipse shape and orientation. Differentiating $\mathbf{L}$ and $\mathbf{A}$ with respect to time, we obtain equations that describe the variation of these quantities due to the action of the magnetic field

$$\frac{d\mathbf{L}}{dt}=-\omega^2[\mathbf{r}\vec{\rho}],\quad \frac{d\mathbf{A}}{dt}=-\omega^2\{[\mathbf{p}[\mathbf{r}\vec{\rho}]]+[\vec{\rho}[\mathbf{r}\mathbf{p}]]\}. \tag{1}$$

As $\omega^2\to 0$, the variation of $\mathbf{L}$ and $\mathbf{A}$ during the rotation period of the electron along the ellipse approaches zero; therefore, the right side of Eqs. (1) can be averaged over the period, assuming that $\mathbf{L}$ and $\mathbf{A}$ are constants in first approximation. The existence of three independent motion integrals follows from the equations obtained after the averaging,

$$L_z,\quad Q=L^2/(1-A^2),\quad \Lambda=4A^2-5A_z^2.$$

L_z is a known, exact motion integral for the hydrogen atom in a magnetic field, and Q and Λ are approximate motion integrals, which are conserved within an accuracy of H^4. The quantity Q is equal to the major semiaxis of the ellipse[4] and its conservation reflects the fact that in first approximation the particles wander along the elliptical trajectories that correspond to the unperturbed energy.

The existence of the motion integrals L_z, Q, and Λ makes it possible to describe analytically the caustic curves and to formulate the Bohr-Sommerfeld quantization conditions. Of the three quantization conditions, two conditions give an obvious result: $L_z=m$ (m is the azimuthal quantum number) and the unperturbed energy $E_0=1/(2Q)=1/(2n^2)$. The third quantization condition, from which the motion integral Λ is determined, is nontrivial. For the formulation of this condition we choose the angle θ between the Runge-Lenz vector and the z axis as the generalized coordinate. The generalized conjugate momentum of this coordinate is the $L_\perp$ component of the angular momentum, which is perpendicular to the plane passing through the z axis, and the Runge-Lenz vector. Using the condition $(\mathbf{L}\cdot\mathbf{A})=0$, we express $L_\perp$ in terms of the motion integrals and the angle θ

$$L_\perp(\theta)=\sqrt{n^2\left(1+\frac{\Lambda}{1-5\sin^2\theta}\right)-\frac{m^2}{\sin^2\theta}}. \tag{2}$$

As a result, the Bohr-Sommerfeld condition assumes the following form:

$$\int_{\theta_1}^{\theta_2} L_\perp(\theta)\, d\theta = \pi (k + 1/2), \tag{3}$$

where θ_1 and θ_2 are the roots of $L_\perp(\theta)$. An important fact here is the presence of a pole inside the square root in Eq. (2) at the points $\pi - \theta_0$ and θ_0 ($\cot \theta_0 = 2$). Because of this, all the trajectories are divided into two nonoverlapping classes: trajectories with $\Lambda < 0$ (it follows from the definition of Λ that $-1 < \Lambda < 4$), which librate within the cone $0 < \theta < \theta_0$ (or $\pi - \theta_0 < \theta < \pi$) and trajectoried with $\Lambda > 0$, which librate outside this cone ($\theta_0 < \theta < \pi - \theta_0$). The energy in first-order perturbation theory, which is expressed in terms of the average value of ρ^2 in the period, is

$$E = E_0 + 1/2\, \omega^2 \overline{\rho^2} = -\frac{1}{2n^2} + \frac{\omega^2 n^2}{4} (n^2 + m^2 + n^2 \Lambda_k). \tag{4}$$

The value of Λ_k is determined from the quantization condition (3).

The motion integral Λ is obtained in a quasiclassical approximation. We can also show that the operator $\hat{\Lambda} = 4\hat{A}^2 - 5\hat{A}_z^2$ commutes with the total Hamiltonian of the system in the n layer at large values of n. In Ref. 5, which was devoted to separating the variables for the hydrogen atom, among the various options we have examined one in which L_z and Λ were chosen as independent motion integrals. Using the results of this paper, we can see that the Schrödinger equation for highly excited states of the hydrogen atom in a magnetic field allows an approximate separation of variables (within an accuracy of H^4) into elliptical-cylindrical coordinates on a sphere in a four-dimensional momentum space. As regards the level splitting at the quasi-intersection point, we should note that the exponential decrease of the splitting with an increase of n is not directly attributable to the existence of an approximate symmetry. This decrease is caused by a separation, which is peculiar to this problem, of the states into two classes ($\Lambda_k < 0$ and $\Lambda_k > 0$), which are localized in two nonoverlapping regions of configuration space in the quasiclassical approximation; therefore, the splitting is determined by the product of the wave functions in the classically forbidden region in which they are exponentially small. The level splitting $\Delta = \langle \psi_1 | V | \psi_2 \rangle$ can be estimated by incorporating the characteristic scale of the Rydberg states in the following way: In the classically forbidden region $\psi_i \sim e^{-r/n}$ we obtain $\Delta \sim \exp(-2n + m)$ by replacing r in the wave function by its average value in the n layer for a constant m. This simple estimate is in good agreement with the results of Refs. 1 and 2. The other matrix elements between the states of the different classes presumably are also exponentially small. This pertains to the oscillator strengths, for which additional approximate selection rules are in effect. If we examine the two states belonging to one class, then the splitting in this case must decrease as a power function with increasing n (presumably as n^{-3}). The obtained results show that in addition to the known separation of states with respect to parity at a constant m, there is an approximate separation associated with the sign of Λ. Four classes of states can thus be identified: ψ_{mg}^{+}, ψ_{mg}^{-}, ψ_{mu}^{+}, and ψ_{mu}^{-} [as usual, the subscripts g and u determine the parity of states, while the superscripts ($\pm$) denote the sign of Λ]. If the superscripts of the two states are different, then the quasi-intersection for these states becomes an exact intersection. For the states in which

only the superscript is different, the splitting is exponentially small for the large parameter n. Finally, if all three indices are identical, the splitting is a power function of n.

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