Quantum and Classical Trajectories in the Hydrogen Atom

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Abstract

The hydrogen atom is the simplest known atom, consisting of a proton and an electron. Its study is important because it makes up a large part of visible matter and, being a simple atom, serves as a basis for understanding atomic structure. Additionally, it is important due to its various applications in industry and as an energy source. From the perspective of quantum mechanics, the hydrogen atom is the only one that allows an exact analytical solution to the Schrödinger equation. This work presents a study of the hydrogen atom using the quantum potential approach. We compute the quantum and classical trajectories for the electron in the hydrogen atom as determined by the eigenfunctions of the following operators: the Hamiltonian, the square of the orbital angular momentum, and the z-component of the orbital angular momentum. In particular, we show the relationship between quantum and classical trajectories, and we also study the intersection between the zeros of the quantum potential and the caustic.

Classical equations

Hamiltonian:

$$H = \frac{1}{2m_e}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 sin^2\theta}\right) - \frac{e^2}{4\pi\epsilon_0\, r}.$$

Hamilton's equations:

$$\dot{r} = \frac{p_r}{m_e},$$

$$\dot{\theta} = \frac{p_\theta}{m_e r^2},$$

$$\dot{\phi} = \frac{p_\phi}{m_e r^2 sin^2\theta},$$

$$\dot{p_r} = \frac{1}{m_e r^3}\left(p_\theta^2 + \frac{p_\phi^2}{sin^2\theta}\right) - \frac{e^2}{4\pi\epsilon_0 r^2},$$

$$\dot{p_\theta} = \frac{p_\phi^2\, cos\theta}{m_e r^2 sin^3\theta},$$

$$\dot{p_\phi} = 0.$$

$\theta = \pi/2$

Hamiltonian:

$$H = \frac{1}{2m_e}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right) - \frac{k}{r}.$$

Hamilton's equations:

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m_e},$$

$$\dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{m_e r^2},$$

$$\dot{p_r} = -\frac{\partial H}{\partial r} = -\frac{-p_\phi}{m_e r^3} - \frac{k}{r^2},$$

$$\dot{p_\phi} = -\frac{\partial H}{\partial \phi} = 0.$$

$$\frac{1}{\tilde{r}} = 1 + \sqrt{1-\alpha}\cos(\phi - Q_2)$$

Where:

$$Q_2 = \pm\phi \pm \int -\frac{p_\phi}{r^2}\left(\frac{1}{\sqrt{-\frac{\mu}{r^2} + 2m_e\left(E + \frac{k}{r}\right)}}\right) dr,$$

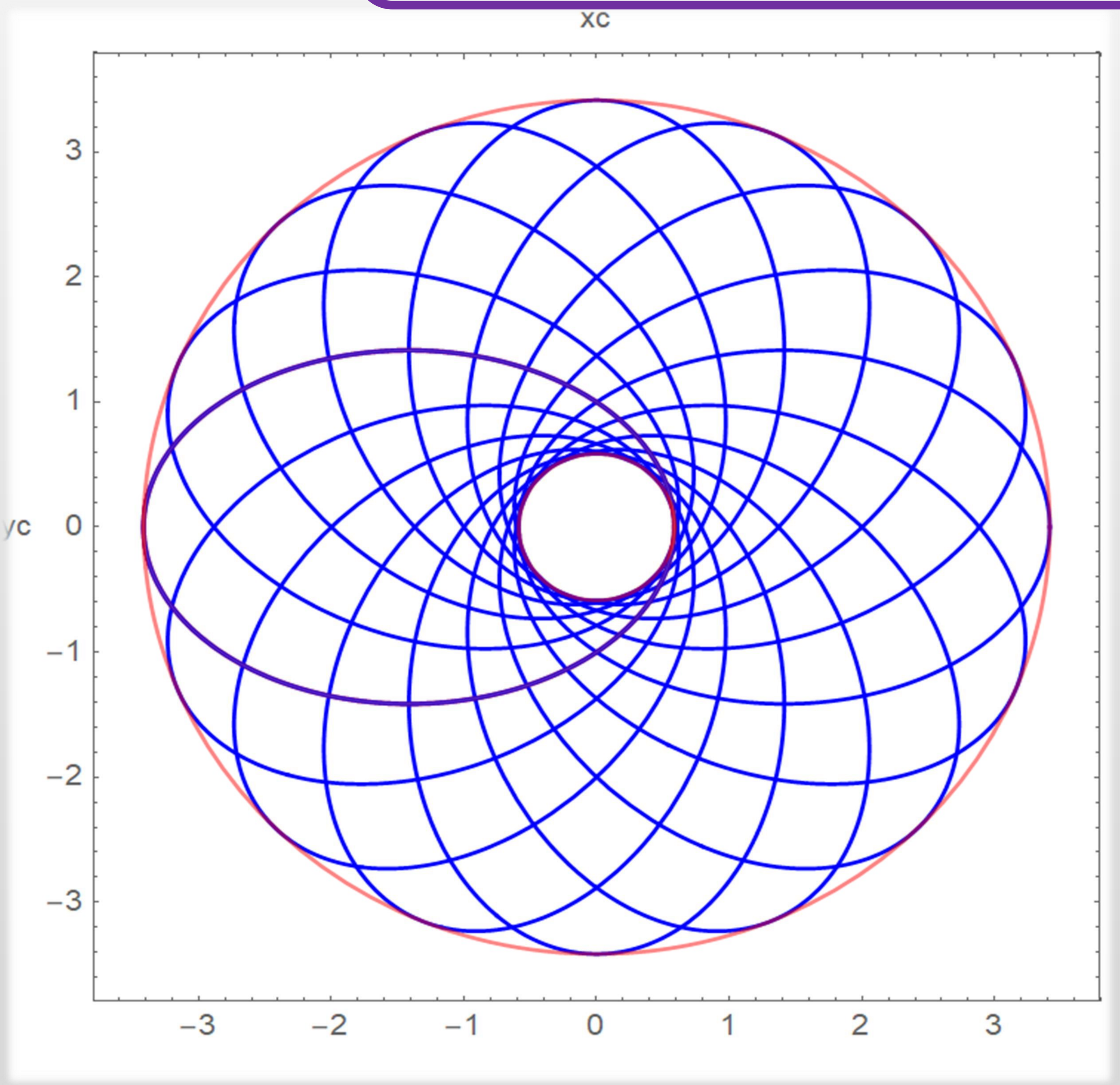
$$\tilde{r} \equiv -\frac{k}{2E_C^0} r,$$

$$E_c = \alpha E_C^0,$$

$$0 < \alpha \leq 1.$$

Caustic region:

$$\tilde{r} = \frac{1}{1+\sqrt{1-\alpha}}.$$



This image shows the trajectory of a particle given by the classical Hamiltonian (blue) and the caustic region (red).

Quantum equations

Schrödinger equation:

$$-\left(\frac{\hbar^2}{2m_e}\right)\nabla^2\Psi - \frac{k}{r}\Psi = i\hbar\frac{\partial\Psi}{\partial t}.$$

Eigenfunctions:

$$\hat{\boldsymbol{H}}\Psi_{nlm}(\boldsymbol{r},t) = E_n\Psi_{nlm}(\boldsymbol{r},t),$$
$$\hat{\boldsymbol{L}}^2\Psi_{nlm}(\boldsymbol{r},t) = \hbar^2 l(l+1)\Psi_{nlm}(\boldsymbol{r},t),$$
$$\hat{L}_z\Psi_{nlm}(\boldsymbol{r},t) = \hbar m\Psi_{nlm}(\boldsymbol{r},t).$$

Wave equation:

$$\Psi_{nlm}(\mathbf{r},t) = R_{nlm}(r,\theta)e^{iS_{nm}(\phi,t)/\hbar},$$

where

$$R_{nlm}(r,\theta) = A_{nlm}\left(\frac{2r}{na}\right)^l e^{-\frac{r}{na}}\left[L_{n-(l+1)}^{2l+1}\left(\frac{2r}{na}\right)\right]P_l^m(\cos\theta),$$

$$S_{nm}(\phi,t) = \hbar m\phi - E_n t,$$

$$a \equiv \frac{\hbar^2}{km_e} = 0.529\times10^{-10}m,$$

$$E_n = -\frac{\hbar^2}{2m_e a^2 n^2} = -\frac{13.6}{n^2}eV.$$

Quantum Hamilton's equations:

$$\dot{r} = \frac{p_r}{m_e},$$
$$\dot{\theta} = \frac{p_\theta}{m_e r^2},$$
$$\dot{\phi} = \frac{p_\phi}{m_e r^2\sin^2\theta},$$
$$\dot{p_r} = \frac{1}{m_e r^3}\left(p_\theta^2 + \frac{p_\phi^2 - m^2\hbar^2}{\sin^2\theta}\right),$$
$$\dot{p_\theta} = \frac{(p_\phi^2 - m^2\hbar^2)\cos\theta}{m_e r^2\sin^3\theta},$$
$$\dot{p_\phi} = 0.$$

Quantum potential:

$$Q_{nlm}(\mathbf{r}) = E_n + \frac{k}{r} - \frac{m^2\hbar^2}{2m_e r^2\sin^2\theta}.$$

Quantum force:

$$\mathbf{F}_{nlm}(\mathbf{r}) = \left(\frac{k}{r^2} - \frac{m^2\hbar^2}{m_e r^3\sin^3\theta}\right)\hat{r} - \left(\frac{m^2\hbar^2\cos\theta}{m_e r^3\sin^3\theta}\right)\hat{\theta}.$$

Conclusions

In this work we have applied the quantum potential approach to study the dynamics of the electron in the hydrogen atom dictated by the stationary states, $\Psi_{nlm}(r,t)$, which are eigenfunctions of the Hamiltonian, square of the orbital angular momentum, and the z-component of the orbital angular momentum operators. We found that each stationary state defines a quantum Hamiltonian system for the electron under the influence of an interaction that is proportional to the eigenvalue, $m\hbar$, of the z-component of the orbital angular momentum operator. In accordance with the quantum potential approach the motion of the electron is given by a subset of solutions to the corresponding quantum Hamilton equations, that subset is singlet out by the condition that the quantum momentum of the electron is given by the gradient of the phase of the wave function.

References

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