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Bohmian picture of Rydberg atoms

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Abstract. Unlike the previous theoretical results based on standard quantum mechanics that established the nearly elliptical shapes for the centre-of-mass motion in Rydberg atoms using numerical simulations, we show analytically that the Bohmian trajectories in Rydberg atoms are nearly elliptical.

Keywords. Rydberg atom; quantum trajectory.

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1. Introduction

Ever since the advent of quantum mechanics one of the fundamental problems in physics has been to elucidate the transition from quantum to classical mechanics. After Schrödinger introduced coherent states in quantum mechanics [1], it became clear that they are optimal quantum mechanical states to describe the classical limit. Recently, there has been a renewed interest in this problem due to the experimental study of Rydberg atoms in external fields which provide a tool to study the quantum-classical transition regime [2,3]. These experiments [4] have shown that the high quantum number states show classical behaviour. Also, higher n values lead to an ever-shrinking energy gap $E_n \propto -1/2n^2$, and the energy spectrum approaches the continuum. Moreover, it is evident [5] that the highest angular momentum state $l = n - 1 = l_n$ in an atom has the special property of being a minimum uncertainty state.

In this paper, we study the problem from the point of view of the de Broglie–Bohm theory [6] to see the relationship between Bohmian trajectories and Kepler orbits in Rydberg atoms.

2. Standard quantum mechanical analysis

It has been shown that wave-packet solutions of the Schrödinger equation for the Coulomb problem travel along classical elliptic orbits of fixed mean eccentricity and angular momentum [5]. These wave-packets are coherent states that have minimal quantum fluctuations in the non-commuting components of the Runge–Lenz vector in the plane of the orbit [7].

The study of the Runge–Lenz vector in quantum mechanics was first undertaken by Pauli [8] who used it to solve the hydrogen atom problem.

In the asymptotic regime of large quantum numbers $n \approx l_0$, the WKB approximation of the radial wave function of the hydrogen atom in 3-dimensions is given by [5]

$$\psi^\delta(r,\theta,\phi,t) \approx \left(\frac{2\omega_0}{\pi p_0(r)}\right)^{1/2} \exp\left[iS_0(r)\right] \left(\frac{\delta l_0}{\pi}\right)^{1/4} \exp\left[-(\theta-\pi/2)^2\frac{\delta l_0}{2}\right]$$
$$\times \sum_{\mu=-\infty}^{+\infty} \exp\left[i\delta l_0(\phi+2\pi\mu) - (\phi+2\pi\mu-\phi_0(r))^2\frac{l_0}{2}(1-\delta^2)\right]$$
$$\times \frac{1}{(2\pi\alpha_0(r,t))^{1/2}} \exp\left[\frac{-\left(\delta(\phi+2\pi\mu-\phi_0(r)) - \frac{t-t_0(r)}{l_0^3}\right)^2}{2\alpha_0(r,t)}\right], \tag{1}$$

where the classical action in radial coordinates is given by

$$S_0(r) = \int^r p_0(r')\mathrm{d}r', \tag{2}$$

with the mean radial momentum

$$p_0(r) = \left(2E_{n_0} - \frac{l_0^2}{r^2} + \frac{2}{r}\right)^{1/2}. \tag{3}$$

In classical mechanics the quantities $\phi_0(r)$ and $t_0(r)$ are related to the action S_0 by

$$\phi_0(r) = -\frac{\partial S_0}{\partial l_0} \text{ and } t_0(r) = \frac{\partial S_0}{\partial E_{n_0}}. \tag{4}$$

The rate of spreading of the wave-packet is given by the complex width

$$\alpha_0(r,t,\delta) = \frac{1}{2\sigma^2} - i\left(\frac{3t}{l_0^4} + 2f_0(r)\right), \tag{5}$$

where $f_0(r) = \partial^2 S/\partial E_n^2$. It follows from eq. (1) that the quantum mechanical phase is

$$S = S_0 + \delta l_0\phi + \frac{1}{2}\arctan(b/a) + \frac{\lambda^2}{4\gamma} - \frac{A^2 b}{2(a^2+b^2)}, \tag{6}$$

where

$$A = \delta(\phi-\phi_0(r)) - \frac{1}{l_0^3}(t-t_0(r)),\ \ \gamma = \frac{2\pi^2 b\delta^2}{(a^2+b^2)},\ \ \lambda = \frac{\pi\delta A}{(a^2+b^2)}, \tag{7}$$

with

$$a = \frac{1}{2\sigma^2} \text{ and } b = \frac{3t}{l_0^4} + 2f_0(r). \tag{8}$$

3. Bohmian mechanical analysis

Let us now examine the problem of coherent states from the perspective of the de Broglie–Bohm theory which is quite close to the classical Hamilton–Jacobi theory. In this theory the quantum mechanical action S given by (6) satisfies the modified Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + Q + V = 0, \tag{9}$$

where

$$Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}, \tag{10}$$

and the wave function, written in the polar form $\psi = R\mathrm{e}^{iS/\hbar}$ satisfies the Scrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\psi. \tag{11}$$

In Bohmian mechanics one introduces the position as an additional variable (the so-called 'hidden variable') through the guidance conditions [9]

$$v_r = \frac{\partial S}{\partial r},\ v_\theta = \frac{1}{r}\frac{\partial S}{\partial\theta},\ v_\phi = \frac{1}{r\sin\theta}\frac{\partial S}{\partial\phi}. \tag{12}$$

Using these conditions, we can readily obtain the Bohmian trajectories of electrons in a Rydberg atom with high l wave-packets provided we also use the result that the radius of the nth Bohr orbit in a hydrogen atom is given by $r_n \approx n^2$. This is the expectation of the radius or its space averaged value. The time averaged value is the same. Using the expression for S given by (6), we finally obtain

$$\begin{aligned}
&\frac{\partial S}{\partial r} = p_0 + \mathscr{O}(l_0^{-7}) + \mathscr{O}(l_0^{-14}),\\
&\frac{\partial S}{\partial\theta} = 0,\\
&\frac{\partial S}{\partial\phi} = \delta l_0 + \mathscr{O}(l_0^{-5}).
\end{aligned} \tag{13}$$

The corresponding expressions in classical mechanics are

$$\begin{aligned}
&\frac{\partial S}{\partial r} = p_0,\\
&\frac{\partial S}{\partial\phi} = \delta l_0,
\end{aligned} \tag{14}$$

and these are known to lead to the equation of an ellipse [10]. Equations (13) and (13) show that the Bohmian trajectories of Rydberg atoms with $l_0 \approx 50$–100 are ellipses for all practical purposes.

4. Concluding remarks

The advantage of the Bohmian analysis we have carried out is that one can see clearly and analytically that the Bohmian trajectories in Rydberg atoms are nearly elliptical. Previous theoretical results using standard quantum mechanics have only been able to establish the nearly elliptical shapes for the centre-of-mass motion using numerical simulations [11].

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References

[1] E Schrödinger, *Naturwissenchafter* **14**, 137 (1927)
[2] R F Stebbings and F B Dunning, *Rydberg states of atoms and molecules* (Cambridge University Press, London, 1983)
[3] G Alber and P Zoller, *Laser excitation of electronic wave packets in Rydberg atoms physics report* **199**, 1 (1991)
[4] J A Yeazell and C R Stroud, *Phys. Rev. Lett.* **60**, 494 (1988)
[5] M Nauenberg, *Phys. Rev.* **A40**, 1133 (1989)
[6] D Bohm and B J Hiley, *The undivided universe* (Routledge and Chapman and Hall, 1993)
[7] C Runge, *Vektoranalysis*, vol. I, p. 70
S Hirzel (Leipzig, 1919)
W Lenz, *Z. Physik* **24**, 197 (1924)
[8] W Pauli, *Z. Phys.* **36**, 336 (1926)
[9] P R Holland, *Quantum theory of motion* (Cambridge University Press, 1993)
[10] H Goldstein, *Classical mechanics* (Addison-Wesley, 1968)
[11] P Bellomo and C R Stroud Jr., *Classical evolution of quantum elliptic states*, arXiv: quant-ph/9812022