

Hydrogen atom trajectories for exact and approximate eigenfunctions

Hannah Anthony and Dr. Isaiah Sumner

Department of Chemistry, James Madison University, Harrisonburg, VA

de Broglie-Bohm theory is a formulation of quantum mechanics that allows us to see that classical, Newtonian mechanics is just a special case of quantum mechanics. In de Broglie-Bohm theory, the wave function is written in polar form ($\Psi(x, t) = A(x, t)e^{-iS(x, t)/\hbar}$) which allows us to separate the time dependent Schrödinger equation into a real and imaginary part. If we set $\bar{\nabla}S$ equal to the momentum of the particle, the real part becomes a classical-like equation of motion that includes a “quantum force” term. The quantum force is responsible for all quantum effects (zero point energy, tunneling, etc). This version of quantum mechanics gives a more intuitive description of the physical system. However, if the particle is in an eigenstate of the Hamiltonian, its wave function is $A(x, t)e^{-iEt/\hbar}$, where E is the particle’s energy. Therefore, its momentum is zero and the particle does not move. However, if the particle also has spin, it is possible to show that the particle’s momentum is non-zero, even in an eigenstate. Thus, we reformulate de Broglie-Bohm theory by taking spin into account and apply it to a hydrogen atom. We tested several methods to integrate the resulting equations of motion. And we present here the results for exact and approximate wave functions.