Rutherford atom in quantum theory

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We predict the existence of a self-sustained one-electron wave packet moving on a circular orbit in the helium atom. The wave packet is localized in space, but does not spread in time. This is a realization *within quantum theory* of a classical object that has been called a ''Rutherford atom,'' a localized planetary electron on an unquantized circular orbit under the influence of a massive charged core.

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There is growing interest in the quantum-mechanical realizations of ''classical'' atoms: atoms with electron wave packets that are fully localized (in three space dimensions) yet do not spread [1]. Such behavior was recently shown to exist for so-called Trojan states, rotating and nonspreading wave packets in hydrogen exposed to a monochromatic circularly or linearly polarized electric field [2–4]. Similar behavior has been shown with the addition of a magnetic field [5]. There are several motivations for studies of such quantum states: They provide an experimental opportunity to study quantum versus classical correspondence [6], quantum softening of classical chaos [7], and possibly even Arnol'd diffusion [8]. Experimental methods now exist to manipulate quantum states of atoms and molecules using strong laser pulses [9] and microwave fields [10], making the generation of fully localized, nondispersing states sustained by external fields a feasible near-future challenge for experimental physics [3].

Nonspreading electron states in bare atoms (without the assistance of external fields) is quite another matter. Such states are superficially and obviously implied by the planetary picture that was first suggested by Rutherford's discovery of massive highly localized nuclei, but they are contradicted by the highly nonlocalized stationary wave functions familiar from elementary quantum theory. However, it was recently shown that nondispersing, fully localized wave packets moving around circular orbits without the assistance of external fields can exist in polar molecules [11]. A class of quasisteady states in bare atoms is known in two-electron atoms [12]. These atomic states correspond to the classical situation in which the inner electron performs rapid linear oscillatory motion near the nucleus. The oscillation of the inner charge generates a stabilizing field for the outer electron, which then remains almost frozen in space [12]. This is called the frozen planet configuration. A nontrivial extension of this phenomenon has recently been discovered [13]. The dynamics of the inner electron on an elliptical orbit can lead to stabilization of circular motion in the outer electron. In that case the outer electron sees the nucleus with charge $Z=2$ but screened by the inner electron as one anisotropic effective charge Z_{eff}, which is significantly less than 1 but neverless provides stabilization of the circular motion. Although the major axis of the inner electron's elliptical orbit adiabatically follows the outer electron, the two electrons orbit the core in opposite directions. When the frequency of the orbital motion of the outer electron approaches zero it reduces exactly to the frozen planet configuration [13].

In this paper we provide the first demonstration of the existence of what has been called [14] a ''Rutherford atom,'' i.e., the wave function for a single electron moving on an unquantized stable and nonspreading planetary orbit about a massive charged core. Such an object would have seemed a much more ''natural'' realization of hydrogen in 1913 compared to Bohr's new quantized atom. Schrödinger and Lorentz later sought to construct such a more natural hydrogen from wave mechanics without success [15].

As we show, in contrast to the polar molecule case [11], a single electron is sufficient to provide a dipole moment capable of stabilizing the atom. Two important differences are that here the outer classical electron plays an active role by polarizing the core, and the system does not reduce to a ''frozen planet,'' as the orbital period of the outer electron gets very large.

We start our analysis from the time-dependent Hartree-Fock equations for a two-electron atom [16] in the Hartree limit,

$$H_i\psi_i = i\frac{\partial\psi_i}{\partial t}, \quad i=1,2 \tag{1}$$

$$H_i = -\frac{\nabla^2}{2} - \frac{2}{|\mathbf{r}|} + \int \frac{\rho_j(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}', \quad i\neq j \tag{2}$$

from which the electron density can be found as

$$\rho(\mathbf{r},t) = \rho_1(\mathbf{r},t) + \rho_2(\mathbf{r},t) = |\psi_1(\mathbf{r},t)|^2 + |\psi_2(\mathbf{r},t)|^2. \tag{3}$$

The exchange potential can be safely neglected since we will seek a split-packet solution, a packet that is spatially localized in two distinct places so that the product $\rho_1(\mathbf{r})\rho_2(\mathbf{r})$ is effectively zero for all values of $\mathbf{r}$. This is obtained if one electron is far from the nucleus (outer component ρ_1) and the other is very near to it (inner component ρ_2).

Our assumption that one electron is near and the other very far from the nucleus allows us retain the dipole term in one of the Hamiltonians [Eq. (2)] and the monopole term in the other. This permits us to look at the Hartree equations (1) as the Schrödinger equations of two separate electrons—one in a Coulomb plus dipole potential with a Hamitonian

$$H_1 = -\frac{\nabla_1^2}{2} - \frac{1}{|\mathbf{r}_1|} + \frac{\mathbf{d}(t)\cdot\mathbf{r}_1}{|\mathbf{r}_1|^3}, \tag{4}$$

and the other in a time-dependent modified Coulomb field with the Hamiltonian

$$H_2 = -\frac{\nabla_2^2}{2} - \frac{2}{|\mathbf{r}_2|} + \frac{1}{|\mathbf{r}_2 - \mathbf{R}(t)|}, \tag{5}$$

where

$$\mathbf{R}(t) = \int \psi_1^*(\mathbf{r}_1,t)\mathbf{r}_1\psi_1(\mathbf{r}_1,t)d\mathbf{r}_1,$$

$$\mathbf{d}(t) = \int \psi_2^*(\mathbf{r}_2,t)\mathbf{r}_2\psi_2(\mathbf{r}_2,t)d\mathbf{r}_2. \tag{6}$$

We consider the case where both **R** and **d** are rotating with the same angular frequency ω,

$$\mathbf{R}(t) = R(\mathbf{x}\cos\omega t + \mathbf{y}\sin\omega t),$$

$$\mathbf{d}(t) = d(\mathbf{x}\cos\omega t + \mathbf{y}\sin\omega t), \tag{7}$$

and then we can linearize the time-dependent terms in Hamiltonians (4) and (5). In the corotating frame, the coupled stationary Hartree equations can be now written as

$$\left[-\frac{\nabla^2}{2} - \frac{1}{|\mathbf{r}|} - E_1 x - \omega L_z\right]\phi_1 = \epsilon_1\phi_1,$$

$$\left[-\frac{\nabla^2}{2} - \frac{2}{|\mathbf{r}|} + E_2 x - \omega L_z\right]\phi_2 = \epsilon_2\phi_2. \tag{8}$$

Here the coupling is via E_1 and E_2, which are effective electric fields defined by

$$E_1 = 2d/R^3, \quad E_2 = 1/R^2. \tag{9}$$

For the outer electron we use our previous result [2,3,17] that in the rotating frame we have a Gaussian packet solution, which in the harmonic approximation can be written as

$$\phi_1(\mathbf{r}) = Ne^{i\omega Ry}e^{-(\omega/2)[Ay^2 + B(x-R)^2]}e^{-(\omega/2)[2iC(x-R)y + Dz^2]}, \tag{10}$$

where A, B, C, and D depend only on the dimensionless parameter $q = 1/R^3\omega^2$,

$$A(q) = \sqrt{(1-q)(8+4q-9q^2-8s(q)}/3q, \tag{11}$$

$$B(q) = s(q)A(q)/(1-q),$$

$$C(q) = [2+q-2s(q)]/3q,$$

$$D(q) = \sqrt{q},$$

and

$$s(q) = \sqrt{(1-q)(1+2q)}. \tag{12}$$

The relative angular confinement of this nondispersing packet can be estimated as $1/(A\omega)^{1/2}R$ and the solution represents a dropletlike electron moving around the circular orbit in the laboratory frame. In the case of the inner electron we will seek a solution in the form of an elliptical state [18] that adiabatically follows the internal field E_2 generated by the outer electron [13]. The average angular momentum of this state is oriented along the angular-momentum vector of the outer electron. In the rotating frame this state can be written in a compact form as a generalized rotation of the circular state $|n_2, n_2-1, n_2-1\rangle$, namely,

$$\phi_2(\mathbf{r}) = \langle\mathbf{r}|e^{-i\alpha A_y}|n_2, n_2-1, n_2-1\rangle, \tag{13}$$

where A_y is the y component of the Runge-Lentz vector **A** for the He^+ ion,

$$\mathbf{A} = \frac{n_2}{2}\left\{\frac{\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}}{2}\right\} - \frac{2\mathbf{r}}{r}, \tag{14}$$

and the parameter α satisfies the condition [13]

$$\tan\alpha = \frac{3n_2E_2}{4\omega}. \tag{15}$$

The dipole moment d for this state can be found analytically as [18]

$$d = \int \phi_2^*(\mathbf{r})x\phi_2(\mathbf{r})d\mathbf{r} = -\tfrac{3}{4}n_2(n_2-1)\epsilon \approx -\tfrac{3}{2}a\epsilon, \tag{16}$$

where we defined $a = n_2^2/2$ as the Bohr radius of the inner electron and $\sin\alpha$ is the eccentricity of this state, related to the average angular momentum,

$$\epsilon = \sin\alpha = \sqrt{1 - \langle L_z\rangle^2/n_2^2}. \tag{17}$$

The equilibrium of forces for the outer electron and the self-consistency of the equations (6), (9), and (15) leads to the following system of equations:

$$1 - q = 3pq\epsilon,$$

$$pq = \frac{8}{9}\frac{\epsilon^2}{(1-\epsilon^2)}, \tag{18}$$

where we have introduced another dimensionless parameter $p = a/R$, which is the ratio between the Bohr radius of the inner state and the radius of the outer packet orbit. Figure 1 shows the parameter p as a function of eccentricity ϵ for q within the limits of harmonic stability [2].

Our Mathieu theory for the wave function ϕ_1 of the outer electron [3] provides the explicit decomposition of this function on aligned hydrogenic eigenstates $\phi_{n,l,l}$,

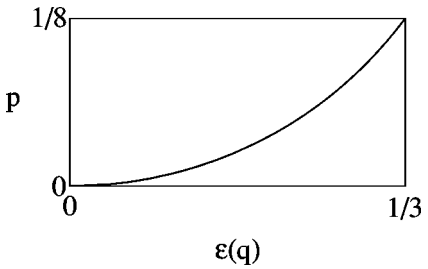

FIG. 1. The ratio p between the inner Bohr radius and the radius of the outer electron orbit as a function of the eccentricity of the inner orbit ϵ. The plot shows ϵ values appropriate to the harmonic stability domain $8/9<q<1$.

$$\phi_1(\mathbf{r})=\sum_n a_n\phi_{n,n-1,n-1}(\mathbf{r}), \tag{19}$$

where the coefficients a_n can be found from the π-periodic zero-order Mathieu function $e_0(\xi,s)$,

$$a_n=\int e_0(\xi,s)e^{-2i\xi(n-n_1)}d\xi, \tag{20}$$

where $n_1^2=\omega^{-2/3}\approx R$ and $s=(4/3)(E_2/\omega^2)$ is the dimensionless parameter in the Mathieu equation for the generating function,

$$\frac{\partial^2 e_0(\xi,s)}{\partial\xi^2}[\mathcal{E}-2s\cos 2\xi]e_0(\xi,s)=0. \tag{21}$$

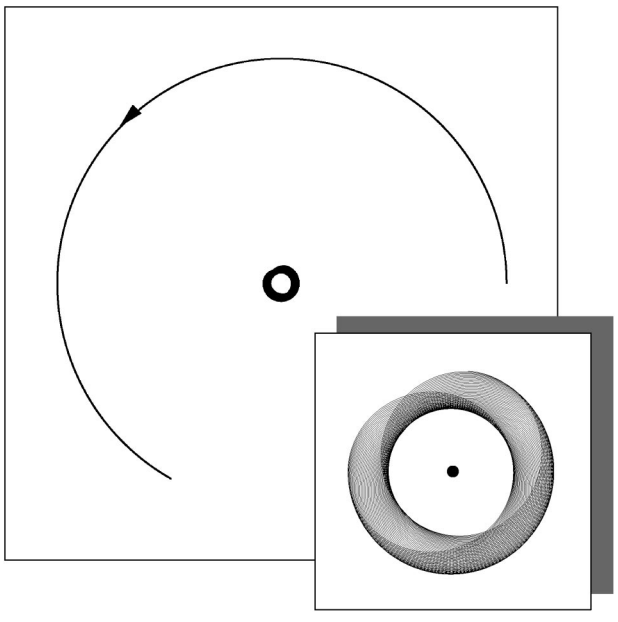

FIG. 2. The classical two-electron orbit in the laboratory frame corresponding to the predicted quantum state for $p=0.061$. The inner electron moves around a nearly circular orbit whose major axis follows the position of the outer electron. In the lower right corner we plot the magnified trajectory of the inner electron.

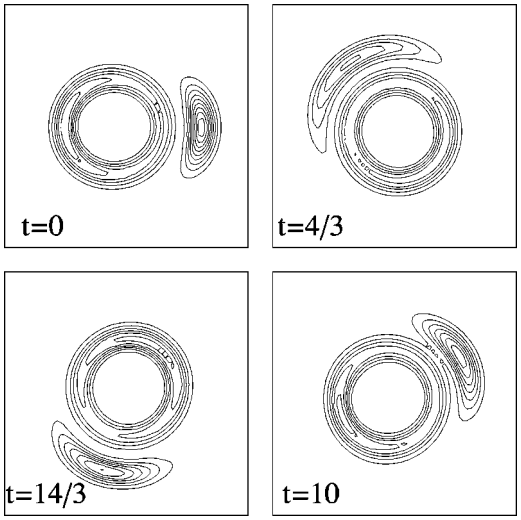

FIG. 3. The stroboscopic snapshots of the time-dependent probability density of the inner and outer electron. The outer electron (Gaussian distribution) is prepared in the Trojan packet state for $n_1=60$ and $q=0.9562$, while the inner electron is in the elliptical state with eccentricity $\epsilon=0.25$ and $n_2=21$. The outer electron is preserved in the Trojan state with some shape oscillations, while the inner follows with the elliptical state polarization. We plot $|\psi_1|^2+0.02|\psi_2|^2$. The outer electron square covers the space region of $10\,800\times 10\,800$ a.u., while the inner is magnified to 1000×1000. The time is in units of cycles of rotation.

Note that the above result cannot be obtained within the perturbation theory [3]. An analogous expansion for the inner electron in the elliptical state in terms of hydrogeniclike states $\Phi_{n,l}$ of He^+ is [19]

$$\phi_2(\mathbf{r})=\sum_{l=-n_2+1}^{l=n_2-1} c_l(\epsilon)\Phi_{n_2,l}(\mathbf{r}), \tag{22}$$

where

$$c_l(\epsilon)=\left[\frac{1}{2^{n_2-1}}\frac{[2(n_2-1)]!}{(n_2+l-1)!(n_2-l-1)!}\right]^{1/2}\left[\frac{1+\sqrt{1-\epsilon^2}}{1-\sqrt{1-\epsilon^2}}\right]^{1/2}\times\epsilon^{(n_2-1)}. \tag{23}$$

Equations (10) and (13) together with Eqs. (18) constitute our final result: namely, the existence of the class of states of helium in which the inner electron is tightly bound to the nucleus, producing a core with a positive charge 1, slightly polarized by the outer electron, which moves around a circular orbit *without spreading*. This solution corresponds to classical solutions in which both classical electrons orbit around the nucleus in the same direction. Figure 2 shows the corresponding classical two-electron orbit of this type. The inner electron is moving around an ellipse with its major axis adiabatically following the circular motion of the outer electron.

It is useful to introduce a natural radius for the outer electron,

$$r_{sc}=R\omega^{2/3}=q^{-1/3}, \tag{24}$$

which is the radius of the outer electron orbit scaled to the Bohr radius for the Kepler frequency ω. For the hydrogen atom, $r_{sc}=1$, and r_{sc} can be used to represent the deviation of the given circular orbit from hydrogenic. For $q=8/9$, which is the border of classical stability of a Trojan state, $r_{sc}=(9/8)^{1/3}\approx 1.0040$. This shows that, for the class of solutions discussed here, the two-electron atom looks almost exactly like a hydrogen atom, but the outer well-localized electron is moving around an unquatized Keplerian circular orbit with frequency ω. Analogous to Trojan states, this state is expected to be a resonant state with a negligible radiative and ionization decay rate ($\Gamma/\omega \approx \alpha_{subt}^3/n_2^2 \rightarrow 0$) if the parameter q is within the interval of harmonic stability [21].

In order to confirm our predictions we have solved the time-dependent Hartree equations (1) and (2) starting with the initial state predicted from our theory and using the inner electron multipole expansion [20]. We applied the split-operator method used in our single-electron simulations [2]. Figure 3 shows the total electron density for both electrons as it develops with time from the predicted state. The outer packet propagates in a well-confined way, while the polarization of the inner state follows.

Summarizing, we have found stable quantum states of two-electron atoms. These are interesting because the atom resembles hydrogen without the quantization restrictions first proposed by Bohr, but requiring the compact nuclear core discovered by Rutherford. Following an earlier convention [14] we call them ''Rutherford atoms.'' Our theory predicts that a subtle adjustment of the state of the inner electron to the state of the outer one must be obtained. The time-dependent mean-field numerical simulations confirmed the existence of our state. The method of preparation of this state will be discussed elsewhere.

Note added. Since submission, reports have appeared that extend in various ways the induced circular stabilization we discovered in Refs. [2,3]. Recent examples are in Ref. [22]

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[1] The emerging topic of ''quantum control'' is concerned with methods of preparing and manipulating well-defined (quasi-classical) quantum states. See, for example, M. Shapiro and P. Brumer, Phys. Rev. Lett. **77**, 2574 (1996); M. Demiralp and H. Rabitz, Phys. Rev. A **55**, 673 (1997).

[2] I. Bialynicki-Birula, M. Kalinski, and J.H. Eberly, Phys. Rev. Lett. **73**, 1777 (1994).

[3] M. Kalinski and J.H. Eberly, Phys. Rev. A **53**, 1715 (1996).

[4] M. Kalinski, J.H. Eberly, and I. Bialynicki-Birula, Phys. Rev. A **52**, 2460 (1995); D. Delande, J. Zakrzewski, and A. Buchleitner, Europhys. Lett. **32**, 107 (1995); J. Zakrzewski, D. Delande, and A. Buchleitner, Phys. Rev. Lett. **75**, 4015 (1995).

[5] E. Lee, A.F. Brunello, and D. Farrelly, Phys. Rev. Lett. **75**, 3641 (1995); A.F. Brunello, T. Uzer, and D. Farrelly, *ibid.* **76**, 2874 (1996).

[6] L.S. Brown, Am. J. Phys. **41**, 525 (1973); J. Mostowski, Lett. Math. Phys. **2**, 1 (1977); J. A Yeazell and C.R. Stroud, Jr., Acta Phys. Pol. A **78**, 253 (1990); Z.D. Gaeta and C.R. Stroud, Jr., Phys. Rev. A **42**, 6308 (1990); Z.D. Gaeta, M.W. Noel, and C.R. Stroud, Jr., Phys. Rev. Lett. **73**, 636 (1994).

[7] A. Buchleitner and D. Delande, Phys. Rev. Lett. **75**, 1487 (1995); M. Holthaus, Chaos, Solitons/Fractals **5**, 1143 (1996); M. Kalinski and J.H. Eberly, Phys. Rev. Lett. **77**, 2420 (1996).

[8] J. von Milczewski, G.H.F. Diercksen, and T. Uzer, Phys. Rev. Lett. **76**, 2890 (1996).

[9] G. Alber, H. Ritsch, and P. Zoller, Phys. Rev. A **34**, 1058 (1986); A. Yeazell and C.R. Stroud, Jr., Phys. Rev. Lett. **60**, 1494 (1988); J.A. Yeazell, M. Mallalieu, J. Parker, and C.R. Stroud, Jr., Phys. Rev. A **40**, 5040 (1990); J.A. Yeazell, M. Mallalieu, and C.R. Stroud, Jr., Phys. Rev. Lett. **64**, 2007 (1990); B. Kohler, V.V. Yakovlev, J. Che, J. L Krause, M. Messina, and K.R. Wilson, *ibid.* **74**, 3360 (1995); D.W. Schumaker, J.H. Hoogenraad, D. Pincos, and P.H. Bucksbaum, Phys. Rev. A **52**, 4719 (1995); M.W. Noel and C.R. Stroud, Jr., Phys. Rev. Lett. **75**, 1252 (1995).

[10] R.G. Hulet and D. Kleppner, Phys. Rev. Lett. **51**, 1430 (1983); J. Hare, M. Gross, and P. Goy, *ibid.* **61**, 1938 (1988); P. Nussenzveig, F. Bernardot, M. Brune, J. Hare, J.M. Raimond, S. Haroche, and W. Gawlik, Phys. Rev. A **48**, 3991 (1993); R.J. Brecha, G. Raithel, C. Wagner, and H. Walther, Opt. Commun. **102**, 257 (1993); C.H. Cheng, C.Y. Lee, and T.F. Gallagher, Phys. Rev. Lett. **73**, 3078 (1994).

[11] I. Bialynicki-Birula and Z. Bialynicka-Birula, Phys. Rev. Lett. **77**, 4298 (1996).

[12] U. Eichmann, V. Lange, and W. Sandner, Phys. Rev. Lett. **64**, 274 (1990); K. Richter and D. Wintgen, *ibid.* **65**, 1965 (1990); V.N. Ostrovsky and N.V. Prudov, Phys. Rev. A **51**, 1936 (1995); V. N Ostrovsky and N.V. Prudov, J. Phys. B **28**, 4435 (1995).

[13] J.A. West, Z.D. Gaeta, and C.R. Stroud, Phys. Rev. A **58**, 186 (1998).

[14] E. Rutherford, Philos. Mag. **21**, 668 (1911). The term ''Rutherford atom'' was introduced by N. Bohr; see A. Hermann, *The Genesis of Quantum Theory (1899-1913)* (MIT Press, Cambridge, MA, 1971), p. 149.

[15] See *Letters on Wave Mechanics*, edited by K. Prizibram (Philosophical Library, New York, 1967), pp. 55–75.

[16] See, for example, K.C. Kulander, Phys. Rev. A **36**, 2726 (1987).

[17] The Trojan stability analysis can be used without modifications only if $d/R \ll 1$, which is the assumption here. Otherwise the higher terms of the dipole moment potential in the Hamiltonian [5] must be included.

[18] W. Pauli, Z. Phys. **36**, 339 (1926); Y.N. Demkov, B.S. Monozon, and V.N. Ostrovskii, Zh. Eksp. Teor. Fiz. **57** 1431 (1970) [Sov. Phys. JETP **30**, 775 (1970)]; D. Delande and J.C. Gay, Europhys. Lett. **5**, 303 (1988); D. Wintgen, Z. Phys. D: At., Mol. Clusters **18**, 125 (1991).

[19] M. Nauenberg, Phys. Rev. A **40**, 1133 (1989).

[20] We solve the full Poisson equation to find the electric field generated by the outer electron while we calculate the inner electron, field up to the dipole moment.

[21] J. Zakrzewski, D. Delande, and A. Buchleitner, Phys. Rev. Lett. **75**, 4015 (1995); Z. Bialynicka-Birula and I. Bialynicki-Birula, Phys. Rev. A **56**, 3623 (1997); see also T.F. Gallagher, *Rydberg Atoms* (Cambridge University Press, Cambridge, England, 1994).

[22] W. Chism and L.E. Reichl, Phys. Rev. A **65**, 021404 (2002); E. Grosfeld and L. Friedland, Phys. Rev. E **65**, 046230 (2002); D.-H. Kwon *et al.*, Phys. Rev. A **65**, 055401 (2002).