Lagrange Equilibrium Points in Celestial Mechanics and Nonspreading Wave Packets for Strongly Driven Rydberg Electrons

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We exhibit analytically and confirm numerically the existence of stable, though nonstationary, quantum states of electrons moving on circular orbits that are trapped in an effective potential well made of the Coulomb potential and the rotating electric field produced by a strong circularly polarized electromagnetic wave. These states are direct counterparts of the Trojans—two clusters of asteroids moving around the Sun in the vicinity of the stable Lagrange points in the Sun-Jupiter two-body system.

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The aim of this Letter is to show that a strong circularly polarized electromagnetic wave with finely tuned parameters will create stable equilibrium points in atoms that are analogous to the gravitational equilibrium points well known in celestial mechanics (cf., for example, [1–4]). Wave packets that describe Rydberg electrons when placed at these points will orbit the nucleus without spreading. Such nonspreading wave packets are direct quantum analogs of the clusters of Trojan asteroids orbiting the Sun near the stable Lagrange points L_4 and L_5 of the Sun-Jupiter system.

Lagrange points $L_1, \ldots, L_5$ are the points of equilibrium in the restricted three-body problem of celestial mechanics at which the centrifugal forces are exactly balanced by the gravitational attraction of the two orbiting bodies. These points have fixed positions in the coordinate frame corotating with the two bodies around their center of mass. The three collinear points lying on the line connecting the centers of the two bodies are unstable. The two equilateral points, lying on the vertices of two equilateral triangles based on the line segment connecting the centers of the bodies, are stable if the mass ratio $\mu = m_2/(m_1 + m_2)$ satisfies the condition $\mu(1 - \mu) < 1/27$. The stability of motion near the equilateral Lagrange points is due to an intricate interplay between the potential forces and the Coriolis force. Essentially the same mechanism is responsible for the stability of motion in the Paul trap. A simple mechanical model with a rotating saddle-shaped potential shown by Paul in his Nobel lecture [5] embodies the essential features of the stabilization mechanism.

The equations describing in the corotating frame the dynamics of a test body oscillating near a stable Lagrange point in the x-y plane defined by the orbiting bodies can be cast into the following general form:

$$dx/dt = p_x + \omega y, \quad dp_x/dt = -a\omega^2 x + \omega p_y, \tag{1a}$$

$$dy/dt = p_y - \omega x, \quad dp_y/dt = -b\omega^2 y - \omega p_x, \tag{1b}$$

where ω is the angular frequency of rotation and a and b are two dimensionless parameters whose values depend on the problem. We have omitted the equations describing the motion in the z direction since this motion decouples from the motion in the x-y plane and is always oscillatory. The two eigenfrequencies ω_+ and ω_- of oscillations in the x-y plane can be found analytically and the oscillations will be stable if both are real. The stability regions in the a-b plane are shown in Fig. 1. Equations (1) are the canonical equations of motion for the Hamiltonian $H_{\rm osc}$ of a harmonic oscillator in a rotating frame,

$$H_{\rm osc} = \frac{p_x^2 + p_y^2}{2} + \frac{a\omega^2 x^2 + b\omega^2 y^2}{2} - \omega(xp_y - yp_x). \tag{2}$$

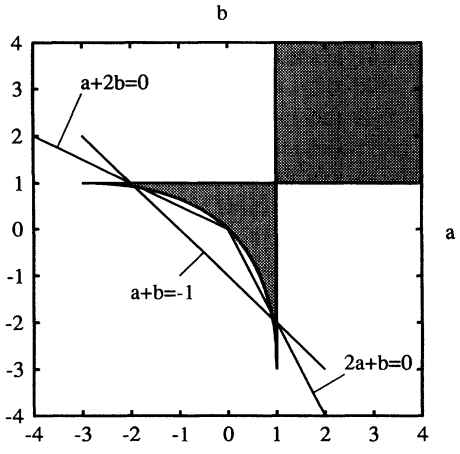

FIG. 1. The islands of stability (shaded areas) in the plane of parameters a and b. In the parabolic triangle the potential has a saddle point but the motion is stable due to an interplay of potential forces and the Coriolis force. Points lying on the three lines intersecting the triangular stability regions correspond to the gravitational three-body problem and to an atom in a circularly polarized wave.

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This expression can be obtained from the full Hamiltonian describing the motion of a test body of mass m in the frame of reference rotating with the angular frequency ω,

$$H_{\rm gr} = \frac{\mathbf{p}^2}{2m} - \frac{Gmm_1}{|\mathbf{r} - \mathbf{r}_1|} - \frac{Gmm_2}{|\mathbf{r} - \mathbf{r}_2|} - \omega(xp_y - yp_x), \tag{3}$$

by expanding the potential around the point of static equilibrium in the corotating frame and keeping only the quadratic terms (the linear terms all cancel out due to the equilibrium condition). This procedure leads for the restricted three-body problem to expressions for the coefficients a and b that are constrained to lie on the line $a + b = -1$ and they belong to the stability island in Fig. 1 if the second mass is either very small compared to the first mass, $\mu < 1/2 - \sqrt{23/108} = 0.038\,52$, or nearly equal, $\mu > 1/2 + \sqrt{23/108} = 0.961\,48$. The mass of Jupiter, slightly less than one-thousandths of the solar mass, meets the first criterion and the two clusters of Trojan asteroids provide a vivid example of the stable equilibrium points in celestial mechanics at work. These asteroids undergo stable oscillations in the rotating frame with the frequencies $\omega_+ = 2\pi/147.4$ yr and $\omega_- = 2\pi/11.9$ yr.

After this brief discussion of stable Lagrange points we can ask about the implications of such an analysis for atomic systems. Are there stable points of equilibrium for atomic electrons that may trap the wave function and produce stable but *nonstationary* states? All we have to do to find such states is to show that Eqs. (1) apply in some situations to atomic systems. The direct analog of the Sun-Jupiter system would be a diatomic molecule with two atoms having the appropriate masses, but the electron clouds screen the forces making the dynamics significantly different from the purely Coulombic case. We found, however, a close analog of a stable Lagrange point in the simple case of a hydrogenlike ion placed in the electric field of a circularly polarized wave. When directed towards the nucleus, the electric field plays the role of the gravitational pull of the lighter body and will lead under the proper choice of parameters to the creation of a stable equilibrium point.

The Hamiltonian for the electron moving in the combined Coulomb and electromagnetic wave field in the rotating frame has the form (in atomic units)

$$H_{\rm el} = \frac{\mathbf{p}^2}{2} - \frac{Z}{|\mathbf{r}|} - \mathcal{E}y - \omega(xp_y - yp_x), \tag{4}$$

where $\mathcal{E}$ is the amplitude of the electromagnetic wave. Note that to derive this expression we only needed to use the dipole approximation in the z direction and that is fully justified. The equilibrium point is on the y axis at a distance y_0 defined by the equilibrium condition:

$$\frac{Z}{\omega^2 y_0^2} - \frac{\mathcal{E}}{\omega^2} = y_0. \tag{5}$$

Note that when $\mathcal{E} = 0$, Eq. (5) is the formula defining the radius of a circular Coulomb orbit and when $Z = 0$ it is the formula for the maximal excursion of a charge in a sinusoidal field, which has been called the Kramers-Hennenberger parameter in recent discussions of atomic stabilization by laser pulses [6]. Upon expanding the Hamiltonian $H_{\rm el}$ around the equilibrium point, we get the Hamiltonian $H_{\rm osc}$ for the motion in the x-y plane with the following identification of the coefficients a and b:

$$a(q) = q, \quad b(q) = -2q, \quad q = Z/\omega^2 y_0^3. \tag{6}$$

The parameter $q = Ze^2/4\pi\varepsilon_0 m\omega^2 y_0^3$ is a characteristic dimensionless parameter in our problem—the ratio of the Coulomb force to the centrifugal force. This parameter approximately corresponds to $1 - \mu$ in the asteroid problem. The values of the parameters a and b for our problem lie on the line $2a + b = 0$ that intersects the boundaries of the stability region at $q = 8/9$ and $q = 1$. It follows from the analysis that the spectrum is indeed real only on the island of stability.

In order to have linear stability in classical mechanics it is sufficient that the initial positions and momenta are sufficiently close to their equilibrium values, but this condition does not guarantee the stability of a quantum mechanical wave packet. Owing to the uncertainty principle a wave packet has a finite extension that must be properly accounted for.

Our quantum mechanical analysis [7] will be based on the Hamiltonian (2) for the oscillator in the rotating frame. The diagonal form of this Hamiltonian is

$$H_{\rm osc} = \omega_+ a_+^\dagger a_+ - \omega_- a_-^\dagger a_-. \tag{7}$$

Note that the second term enters with a minus sign. Thus, the Hamiltonian is not bounded from below, but it still has a complete set of square integrable states. These states are stable within the present approximation. Transitions between these states are caused by the nonlinear corrections to the Hamiltonian (2) and by the spontaneous emission of photons. The transition rates for these processes will be small if we can make the wave packet small. The Gaussian wave packet describing the fundamental state annihilated by both annihilation operators a_+ and a_-—the analog of the vacuum state—is described by the following wave function:

$$\psi_0(x, y) = Ne^{-i\omega x y_0} e^{-\frac{\omega}{2}\left[Ax^2 + B(y - y_0)^2 - 2iCx(y - y_0)\right]}, \tag{8}$$

where A, B, and C are the following functions of q:

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

$$B(q) = \sqrt{(1 + 2q)[8 + 4q - 9q^2 - 8s(q)]}/3q, \tag{10}$$

$$C(q) = [2 + q - 2s(q)]/3q, \tag{11}$$

and $s(q) = \sqrt{1 + q - 2q^2}$. The real parts of these functions are depicted in Fig. 2. Within the region of stability all three functions are real and A and B are positive. Even for the largest value of A, the wave packet is still almost 3 times more compressed in the y direction (parallel to the electric field in the rotating frame) than in the x direction. This means that in the laboratory frame the angular dimensions of the rotating wave packet are bigger than its radial dimensions. We have found that the best (largest) possible value of A, $A = 0.0627$, is obtained when $q = q_b = 0.9562$, roughly in the middle of the stability region. The corresponding values of the remaining parameters are $B = 0.5115$ and $C = 0.7816$. These values correspond to the maximally localized wave packet. The value of the electric field corresponding to q_b obtained from the equilibrium condition is

$$\mathcal{E} = -\omega^{4/3}(1 - q_b)(Z/q_b)^{1/3} = -0.044\,42(Z\omega^4)^{1/3}. \tag{12}$$

In order to satisfy the conditions for the validity of our approximations, the extension of the wave packet in the (critical) x direction measured by $1/\sqrt{\omega A}$ must be much smaller than the radius $y_0 = (Z/q\omega^2)^{1/3}$ of the orbit, leading to the condition

$$\omega \ll Z^2A^3/q^2. \tag{13}$$

For the best value of q and for $Z = 1$ we obtain $\omega \ll 10^4$ GHz, so that the upper boundary of the frequency is in the range $\omega \approx 100$–200 GHz and the corresponding field amplitude is $\mathcal{E} \approx 800$–2000 V/m. Since $q_b \approx 1$, even for the strong field the radius of the orbit in the presence of the field is not much different from its value for the same frequency when there is no field present. Thus we can introduce an effective quantum number n defined by the formula $y_0 = n^2/Z$, which relates the radius of the orbit y_0 to the principal quantum number for high Rydberg states [8]. However, we emphasize that the familiar n, l, m basis is not at all appropriate here, and an expansion of our wave function in that basis will contain many terms with comparable amplitudes. In terms of n the condition (13) becomes $n \gg \sqrt{q}/A$ which for $q = q_b$ gives $n \gg 15.6$ independent of Z. Thus our picture of electrons moving steadily around the nucleus in the field of the circularly polarized wave is well justified only for sufficiently large orbits, whose radii have more than 10^4 atomic units. For $\omega = 200$ GHz and for hydrogen we obtain the field amplitude $\mathcal{E} = 1930$ V/m and the effective quantum number $n = 60$. These conditions may not be very difficult to achieve, and the main experimental problem in observing the atomic stability islands will be to assemble the electron wave packet with the right characteristics.

Our conclusions are fully supported by numerical simulations. We have solved numerically the initial value problem for the two-dimensional Schrödinger equation in the laboratory frame, using a 512×512 grid and well-tested techniques [9]. The initial wave function was chosen in the form (8). In Fig. 3 we show snapshots of packet probability contour lines at various values of time. In Fig. 4 at full-cycle intervals we plot the percentage of the packet probability that falls inside the same rectangular grid that held 70% of the packet probability at $t = 0$. After a decrease in the first one or two orbits, this probability stabilizes around 50%, with fluctuations due to spatial deformations that arise from the nonadiabatic initiation.

In conclusion, we have shown that in the presence of circularly polarized electromagnetic waves there exist classically stable but nonstationary states of electrons in atoms. In quantum theory these are approximately described by Gaussian wave packets which must satisfy

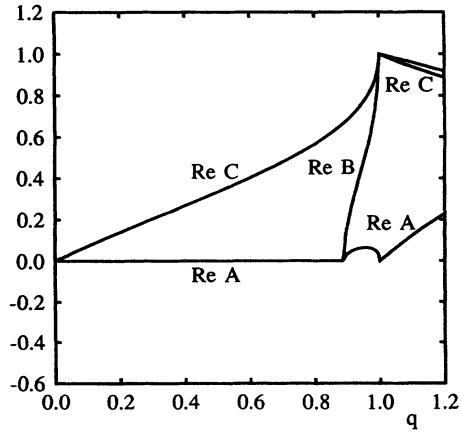

FIG. 2. Real parts of the Gaussian parameters A, B, and C plotted as functions of the parameter q. Note that the real part of A is much smaller than the real part of B in the stability region $8/9 < q < 1$.

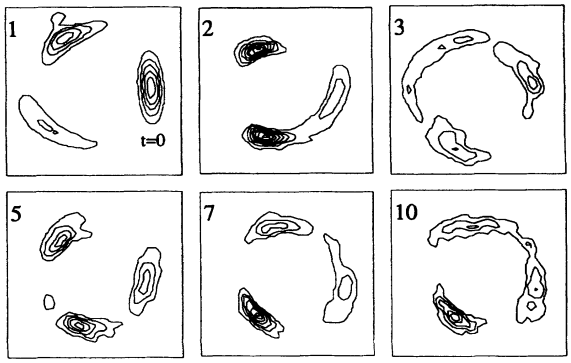

FIG. 3. Time evolution of the wave packet in the laboratory frame. Snapshots of the contour lines of the probability distribution are taken 3 times per cycle for the cycles 1, 2, 3, 5, 7, and 10. The packet starts with the smooth Gaussian shape shown in cycle 1 and moves counterclockwise.

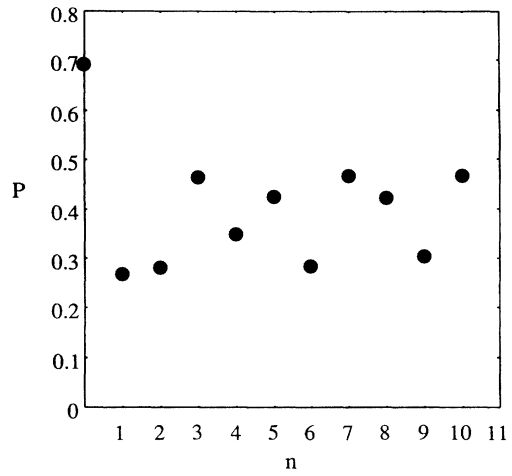

FIG. 4. Values (computed at the end of the nth orbit) of the packet probability. We included all of the packet that lies inside the same rectangle that holds 70% of the total probability at $t = 0$.

(13) to remain nonspreading, a condition that begins to be satisfied in the range $n \approx 50-100$ of effective principal quantum number. These nonspreading wave packets, although formally similar to quantum wave packets on Kepler orbits studied theoretically and experimentally before [8,10], are quite special. They are held together in dynamic equilibrium by a combination of the Coulomb force and the rotating electric field. In order to achieve this special stability, fine tuning of the parameters of the wave is necessary. Although the required electric field is quite strong in atomic units, the effect studied here is distinct from the strong laser stabilization discussed recently [6] because in the present case the Coulomb force is fully included in determining the size of the stabilized orbit. As our numerical solutions show, even in the region around $n \approx 60$, the stability remains quite strong, in the sense that packet probability does not appreciably decay over many orbits. However, the packet does exhibit quasiperiodic deformations, showing that nonlinear effects can be important. We expect to discuss these in detail elsewhere. The spreading of Rydberg wave packets, originating primarily from classical causes, as discussed by Nauenberg [10], does not occur in our case—after all the Trojan asteroids do form stable clusters.

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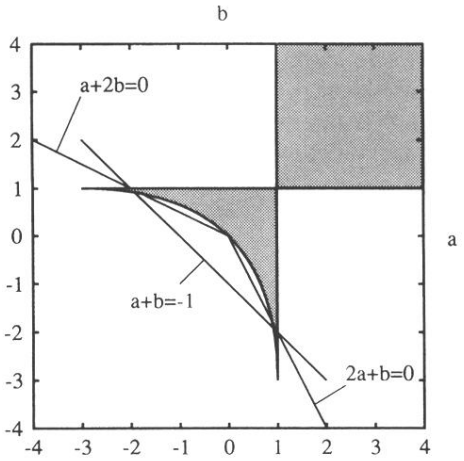

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