Single Atom Quasi-Penning Trap

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The combination of a circularly polarized microwave field and a magnetic field can be used to create a global equilibrium point—an outer minimum—in the electronic dynamics of Rydberg atoms. Stable motion can be maintained at this minimum and the Rydberg electron is localized both radially and angularly while moving on a circular Kepler orbit in a region of space that excludes the nucleus.

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Earnshaw's theorem [1] precludes the possibility of trapping a charged particle in free space solely by using a combination of static electric fields. The development of ion and electron traps has, therefore, relied on the combinations of static electric and radio-frequency fields (Paul trap [2]) or static electric and magnetic fields (Penning trap [3]) [4]. Some time ago Clark, Korevaar, and Littman [5] proposed the possibility of a single Rydberg atom functioning as a quasi-Penning (QP) trap; the system suggested was a hydrogen atom subjected to crossed electric and magnetic fields—the $\mathbf{E} \times \mathbf{B}$ problem—for which long-living resonances associated with the Stark saddle point were predicted [5]. However, the spectral signature expected from the QP orbits has not, so far, been detected [6,7].

In this Letter we propose an alternative: We show that by combining a circularly polarized (CP) microwave field with a homogeneous magnetic field it is possible to confine a Rydberg electron both angularly and radially while the wave packet moves on circular orbits lying beyond the Stark saddle point. Technically this corresponds, perhaps, most closely to an analog of the so-called combined trap [8]. However, in a frame rotating with the CP field frequency the system resembles an atom in crossed electric and magnetic fields and may, therefore, be considered to constitute a microscopic QP or Rydberg atom trap (RAT). Although Rydberg atoms in either magnetic [9] or CP [10] fields have already been well studied theoretically and experimentally, the effect of the combination of the two fields has apparently not previously been considered [11].

In atomic units the Lagrangian for a hydrogen atom subjected to crossed CP and magnetic fields (denoted CP $\times$ **B**) in the dipole approximation is given by

$$\mathcal{L} = \frac{\dot{x}^2 + \dot{y}^2 + \dot{z}^2}{2} + \frac{1}{r} - \frac{\omega_c}{2}(x\dot{y} - y\dot{x}) - F(x\cos\omega_f t + y\sin\omega_f t), \quad (1)$$

where the magnetic field is taken to lie along the positive z direction. In Eq. (1) ω_c is the cyclotron frequency, ω_f is the CP field frequency, and F is the field strength. At this point it is useful to go to a frame rotating with the CP frequency which eliminates the explicit time dependence in Eq. (1), producing the Hamiltonian [12]

$$H = K = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) - \frac{1}{r} - \left(\omega_f - \frac{\omega_c}{2}\right)(xp_y - yp_x) + \frac{\omega_c^2}{8}(x^2 + y^2) + Fx, \quad (2)$$

where K is the Jacobi constant. No change of notation has been made and all coordinates are now assumed to refer to the rotating frame. The key point is that the coefficient in the paramagnetic or linear Zeeman (LZ) term—a Coriolis-like term—in Eq. (2) may be "tuned" by varying ω_c and ω_f. It is interesting to note that a similar strategy has been employed by Ramsey in his work on magnetic shielding of nuclei in molecules [13]—see also [14–17].

The presence of a velocity dependent term makes it no longer possible to define a potential energy surface. However, the role of the paramagnetic term may be uncovered by constructing a zero-velocity surface (ZVS), or effective potential. The use of zero-velocity surfaces is widespread in celestial mechanics [18] and has recently found application in atomic and molecular physics [19–21]. The effective potential or ZVS for the CP $\times$ **B** system is given by

$$V = H - \frac{\dot{x}^2 + \dot{y}^2 + \dot{z}^2}{2} = -\frac{1}{r} + \frac{\omega_f(\omega_c - \omega_f)}{2}(x^2 + y^2) + Fx. \quad (3)$$

Before proceeding it is useful to consider two particular limits.

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(i) In the $\mathbf{E} \times \mathbf{B}$ limit $\omega_f = 0$, the effective potential is

$$V = -\frac{1}{r} + Fx. \tag{4}$$

The ionization threshold is given by the simple Stark saddle point (SSP) criterion [5,7,22,23], and classically, ionization is possible—but, unlike in the pure Stark effect, not inevitable [21]—whenever the energy exceeds the energy of the saddle point. Note that no outer equilibrium point can exist in the effective potential [24].

(ii) The pure CP (i.e., $\omega_c = 0$) problem is more complicated: The effective potential is given by

$$V = -\frac{1}{r} - \frac{\omega_f^2}{2}(x^2 + y^2) + Fx \tag{5}$$

and the electron may escape if its energy lies above the saddle point in the ZVS, although above threshold, bound, classical motion is also possible [19]. However, the ionization mechanism in the CP case is considerably more intricate than for the $\mathbf{E} \times \mathbf{B}$ problem, involving destabilization of a maximum in the effective potential through a Trojan bifurcation [19,25].

The CP $\times$ $\mathbf{B}$ system differs considerably from these two limits in that the coefficient of the term in $x^2 + y^2$ in the ZVS can be arranged to be nonzero and positive. This occurs whenever $\omega_c - \omega_f > 0$ provided that $\omega_f \neq 0$. For a given ω_c this coefficient is maximized when $\omega_f = \omega_c/2$, i.e., the LZ tern in Eq. (2) is absent, and the ZVS becomes equivalent to the potential energy surface (this case is illustrated in Fig. 1). Clearly, the electron can ionize only along the z direction even though this is *not* the electric field direction (in the rotating frame). The ionization threshold is given by $E_{\text{ion}} = -F^2/2\omega_f(\omega_c - \omega_f)$, which may lie above or below the saddle point depending upon the particulars of the fields. In any case, the combination of a time dependent microwave field and a magnetic field causes the dynamics to differ greatly from either the pure Stark effect or the $\mathbf{E} \times \mathbf{B}$ system.

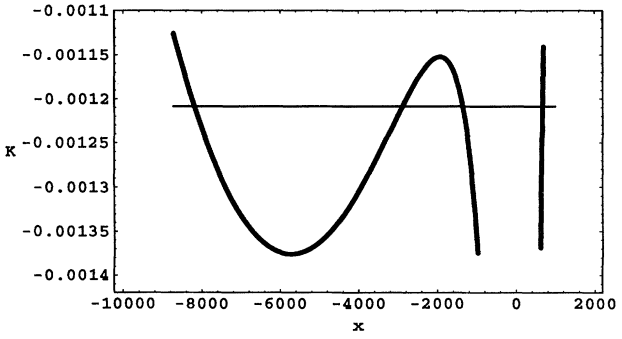

FIG. 1. Section through the ZVS ($y = 0$) with $\omega_c = 3.72$ T, $\omega_f = 52.07$ GHz, and $F = 2000$ V/cm. These parameters correspond to $\omega_f/\omega_c = 1/2$. The horizontal line shows the ionization threshold for the 3D problem—in the planar limit the system cannot ionize.

In this Letter we consider only the case $\omega_f < \omega_c$ because the situations with $\omega_f = \omega_c$ and $\omega_f > \omega_c$ are essentially equivalent to the $\mathbf{E} \times \mathbf{B}$ and CP problems, respectively: Both of these systems have already been studied extensively. We examined the stability of the critical points of the ZVS and found that a transition occurs at $F_c = 3[\omega_f(\omega_c - \omega_f)]^{2/3}/\sqrt[3]{4}$: For $F < F_c$ the ZVS possesses no real critical points. At $F = F_c$ a real, double critical point is spawned that, with increasing F, splits into a saddle point and a minimum, as revealed by a stability analysis of the Hamiltonian flow [19,25].

Figure 1 is a section ($y = z = 0$) through the ZVS and shows clearly the existence of both a saddle point and a minimum in the effective double-well potential together with the ionization energy for these parameter values. The equilibrium point is stable and corresponds to a global minimum—indeed Taylor expansion to second order at the minimum shows that (a) the motion in the x-y plane separates from that in the z direction and (b) the electron may be globally confined in all three degrees of freedom at this fixed point provided the energy in the rotating frame lies below the ionization energy. Of course, the depth of the well and its proximity to the nucleus depend sensitively on the field strengths. Figure 2 shows the projection onto the plane of a typical wave function $\Psi(x, y)$ obtained by numerical diagonalization (using a harmonic oscillator basis) about the minimum whose principal contribution is from the separable state with oscillator quantum numbers

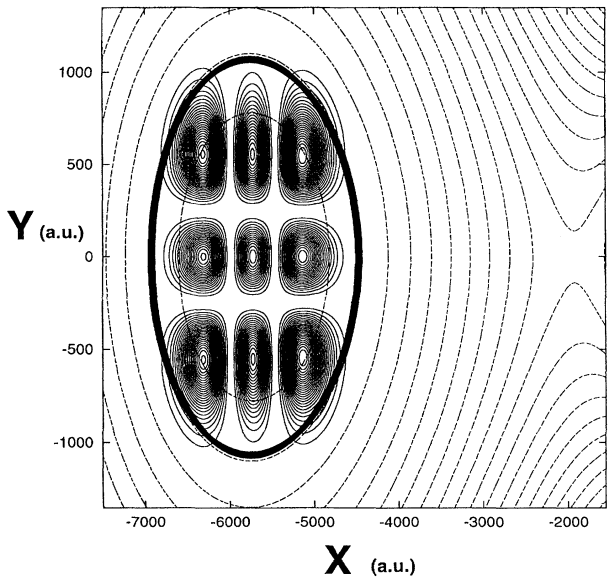

FIG. 2. Level curves of the ZVS for the same parameters at Fig. 1. Superimposed are contours of the wave function whose principal component has $n_x = n_y = 2$ as obtained by numerical diagonalization of a high order Taylor expansion at the minimum. The energy of this state is ≈ -0.00134 a.u. (shown by the thick contour), which falls significantly below the ionization threshold.

$n_x = n_y = 2$. This figure gives an idea of the relative sizes of the wavelength of the electron and the thickness of the barrier between the well and the nucleus. Associated with the equilibrium point is a *family* of nonstationary, nondispersive eigenstates, each of which constitutes a new type of quantum mechanical state. These states are direct analogs of the Trojan wave packet described in Ref. [26]: Indeed, a family of such eigenstates will similarly exist at a stable maximum, thereby generalizing the concept of a Trojan wave packet [11,26].

The equilibrium point at the minimum in the ZVS is similar to the Lagrange equilibrium point in the CP problem [19,26] in that, in the nonrotating frame, it corresponds to a large, stable, circular orbit. However, the CP equilibrium is associated with a *maximum* in the ZVS of Eq. (5), whereas the equilibrium point lying to the left of the saddle in Fig. 1 is a true minimum. In the pure CP case the maximum can be destabilized via a Trojan bifurcation (induced, e.g., by increasing the field strength [19]). The absence of confining potential walls at a maximum means that after the Trojan bifurcation, the electron can escape from the vicinity of the equilibrium point [27]; i.e., chaotic trapped motion at the maximum is not possible [11]. In contrast, at the minimum, the motion will always be confined within the well provided (i) the well exists, (ii) the well is deep enough to support bound states (of course escape through tunneling may be possible but this will be relatively unimportant for large n values), and (iii) escape along the z direction is prevented by choosing an energy below $E_{\rm ion}$. In contrast to the maximum, chaotic trapped motion at the minimum is possible and this situation will be discussed more fully elsewhere. It is reasonable to conclude, therefore, that associated with the stable minimum in Fig. 1 will be stable nonspreading localized 3D wave packets that move along circular orbits well removed from the nucleus. For parameter values for which the well is close to being harmonic, these wave packets will approximate nonspreading, nondispersive coherent states.

In examining the dynamics further it is convenient to scale coordinates and momenta; $\mathbf{r}' = \omega_c^{2/3}\mathbf{r}$, $\mathbf{p}' = \omega_c^{-1/3}\mathbf{p}$. After dropping the primes this yields the Hamiltonian

$$H = \mathcal{K} = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) - \frac{1}{r} - \left(\Omega - \frac{1}{2}\right)(xp_y - yp_x) + \frac{1}{8}(x^2 + y^2) + \epsilon x, \quad (6)$$

where $\mathcal{K} = K/\omega_c^{2/3}$, $\Omega = \omega_f/\omega_c$, and $\epsilon = F/\omega_c^{4/3}$. This scaling shows that the dynamics depends only on the three parameters $\mathcal{K}$, Ω, and ϵ. For convenience we exploit the fact that initial conditions that are confined to the x-y plane (i.e., $z = p_z = 0$) will remain in that plane [12], thus allowing the construction of Poincaré surfaces of section. Figure 3(a) is a typical surface of section for a value of $\mathcal{K}$ midway between the minimum and the saddle point. The figure clearly shows stable motion localized in the well in the ZVS. Interestingly, for the special value of $\Omega = \frac{1}{2}$ (i.e., paramagnetic term absent) in Fig. 3(b), the dynamics in the well is essentially harmonic and the motion appears to be almost integrable—this is reasonable given that, at relatively large distances from

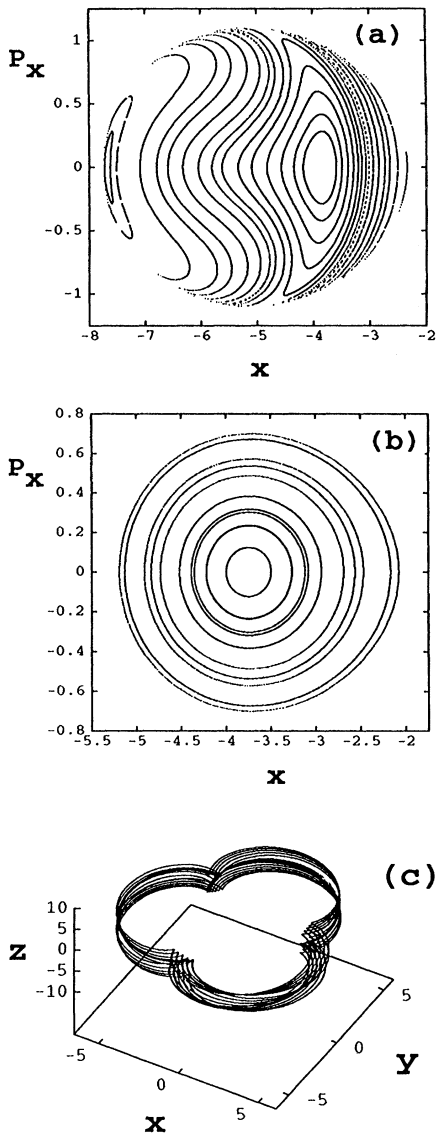

FIG. 3. Composite surfaces of section (integrations in regularized parabolic coordinates) and $\epsilon = 1$; (a) $\Omega = 0.75, \mathcal{K} = -2.25$; (b) $\Omega = 0.05, \mathcal{K} = -1.95$; and (for different initial conditions) (c) typical trajectory integrated in the *nonrotating* frame corresponding to an initial condition started in the ZVS well with $\Omega = 0.25$. In (a) and (b) structure around the origin has been omitted for clarity.

the nucleus, the Hamiltonian (6) is almost separable when $\Omega = \frac{1}{2}$. However, calculations of harmonic generation spectra in Ref. [13] for a similar Hamiltonian point to the nonseparability of the system since nonseparability is necessary for high order harmonic generation.

Figure 3(c) shows a *typical* trapped trajectory in the nonrotating frame obtained by direct integration of the Hamiltonian corresponding to Eq. (1), i.e., including motion in the z direction. It is apparent that stable trapped motion associated with the well in the two-dimensional ZVS is possible in the full-dimensional system, and this is borne out by extensive classical simulations provided that one works below the ionization threshold exemplified in Fig. 1. In practice the ionization threshold is quite sensitive to the actual parameters, much more so than the depth of the well itself, providing the flexibility to adjust the experimental parameters needed to trap a substantial population in the well. The system thus constitutes a RAT for the electron. At energies above the saddle point and for the parameter values in Fig. 3, chaotic motion is possible, coexisting with regular, localized motion around elliptic fixed points originating in the well. Time dependent quantum simulations are underway to investigate further the ramifications of our findings. Finally we note that our results also apply to the problem of an exciton in crossed fields—in this situation genuinely two-dimensional states can be prepared by physical confinement to thin layers in semiconductor materials [16]

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