Axial to transverse energy mixing dynamics in octupole-based magnetostatic antihydrogen traps

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Abstract

The nature of the trajectories of antihydrogen atoms confined in an octupole minimum-B trap is of great importance for upcoming spectroscopy, cooling, and gravity experiments. Of particular interest is the mixing time between the axial and transverse energies for the antiatoms. Here, using computer simulations, we establish that almost all trajectories are chaotic, and then quantify the characteristic mixing time between the axial and transverse energies. We find that there are two classes of trajectories: for trajectories whose axial energy is higher than about 20% of the total energy, the axial energy substantially mixes within about 10 s, whereas for trajectories whose axial energy is lower than about 10% of the total energy, the axial energy remains nearly constant for 1000 s or longer.

1. Introduction

Motivated by testing fundamental symmetries between matter and antimatter, physicists have long been interested in studying the properties of antihydrogen atoms. Of particular interest have been studies of charge-parity-time invariance and the weak equivalence principle. Since first trapping antihydrogen in 2010 [1], the ALPHA collaboration at CERN has measured the antiatom’s microwave spin flip frequency [2], set crude limits on their acceleration in earth’s magnetic field [3], measured their charge to better than 1 ppb and set a new, similarly precise limit on the positron charge anomaly [4], and began measurements of their 1S–2S [5] and hyperfine [6] spectra.

Antihydrogen atoms have a non-zero magnetic moment $\mu_B$, and ALPHA takes advantage of this moment to trap the antiatoms in a minimum-B trap [7]. The trap confines those antiatoms whose magnetic moment is aligned such that they are attracted to the minimum of the trap magnetic field $B$, and whose kinetic energy is below the trap well depth, $\mu_B \left( |B_{\text{wall}}| - |B_{\text{center}}| \right)$, namely the moment times the difference in the magnitude of the magnetic field between the trap wall and the trap center. In ALPHA’s trap (see figure 1), this magnetic minimum is created by an octupole magnet which produces transverse fields of magnitude 1.54 T at the trap wall ($R_{\text{wall}} = 22.3$ mm), and five evenly-spaced mirror coils which produce axial fields of up to 1 T at their centers. The most distant mirror coil centers are symmetrically located at distances $z = \pm 137$ mm from the trap center at $z = 0$. The octupole and mirror fields are superimposed on a uniform axial field of 1 T produced by an external solenoid [8, 9]; taken together, these magnets create a trap of depth $\sim 540$ mK [3]. (Here and throughout, we use kelvin as an energy unit.) Note that while we use the parameters of the ALPHA experiment herein, our results apply, qualitatively, to other minimum-B antihydrogen traps [10], and, more distantly, to neutron traps [11–14].

The antiatom trajectories in an octupole-based minimum-B trap are analytically intractable [16], and must be studied numerically. In this paper, we begin with a discussion of our numeric trajectory simulations, and then prove that the antiatom trajectories are chaotic. Next, we investigate the time it takes for the parallel energy, $E_z$, and transverse energy, $E_\perp$, to mix. (Parallel and transverse are defined relative to the trap axis in the $\hat{z}$ direction.) We find that for a majority of the trajectories, the mixing time is short, i.e., less than approximately 10 s, but for a substantial fraction of the trajectories, the mixing time is very long, i.e., greater than 1000 s.
Knowledge of this parallel to transverse energy mixing time is useful for many current and planned experiments. For example, the mixing time partially determines the fractional time that antiatoms are exposed to light in a small-volume optical cavity centered on the trap axis; it is possible for the antiatoms to gain so much transverse energy that they rarely traverse this axis. The mixing time sets limits on gravity experiments which plan to balance gravity with a magnetic gradient; mixing between the different forms of energy upsets the balance. In both these cases, energy mixing is potentially detrimental to the experimental goals. However, laser cooling of antiatoms with a near-axis laser beam\[17\] relies on mixing to cool the transverse dimensions; here, mixing is beneficial. Likewise, adiabatic expansion cooling benefits from mixing. Thus, while all these phenomena are complicated, and the mixing time is not the sole important factor, knowledge of the mixing time informs the experimental designs.

2. Simulations

The Hamiltonian of a single antihydrogen atom confined in ALPHA’s magnetic trap is given by:

$$\mathcal{H}(x, p) = \frac{p^2}{2M} - \mu_B \cdot B(x),$$

where \((x, p)\) are the coordinates in six dimensional phase space \((x, y, z, px, py, pz)\), and \(M\) is the mass of the antihydrogen atom. As the trap only confines low-field seeking atoms whose magnetic moments are aligned anti-parallel to the local magnetic field, the potential term \(U(x) = -\mu_B \cdot B(x)\) can be simplified to \(\mu_B |B(x)|\). (Magnetic moments do not spontaneously flip in our trap.) Thus, we will work with the reduced equation

$$\mathcal{H}(x, p) = \frac{p^2}{2M} + \mu_B |B(x)|.$$

The magnetic field \(B(x)\) in equation (2) is conveniently split into three components,

$$B(x) = B_{\text{mir}}(x) + B_{\text{oct}}(x) + B_{\text{sol}}(x),$$

where \(B_{\text{mir}}, B_{\text{oct}}, B_{\text{sol}}\) are the fields from the mirror, octupole, and solenoids magnets respectively. In our simulation, we use an approximate analytic model for these fields as described in appendix A and in [18].

For an ideal octupole, \(B_{\text{oct}}(x)\) contains complementary radially- and azimuthally-directed components only, and \(|B_{\text{oct}}(x)|\) is a function of the radius only. If we ignore the radial components of \(B_{\text{mir}}(x)\), then \(|B(x)|\) would be independent of the azimuthal angle \(\theta\). Thus, the potential in equation (2) would be azimuthally symmetric, and the Hamiltonian would conserve angular momentum. The Hamiltonian would then separate, and the orbital dynamics would be simple. However, \(B_{\text{mir}}(x)\) does contain radially-directed components. These radially-directed components mix with those from \(B_{\text{oct}}(x)\), and this mixing breaks the azimuthal symmetry. Angular momentum is not conserved and the dynamics are complicated. Among other effects, these radial terms, which are particularly strong off-axis near the ends of the trap, mix the axial and transverse energies.

We use a symplectic integrator to solve equations (2) and (3). The step size used in the integrator was chosen to be small enough that ensemble-averaged statistical measures converge to well better than 1%. All simulations begin by launching antiatoms from locations drawn from an ellipsoid of radius 0.8 mm and length 16 mm. This volume corresponds to the volume of the positron plasma in ALPHA. Antihydrogen is formed, presumably by three body recombination, when antiprotons transit this volume. Before antihydrogen formation, the antiprotons are assumed to equilibrate with the temperature of the positron plasmas [19, 20]. Hence, the resulting antiatoms are created at this same temperature. However, the positron temperature is much greater.
than the well depth, and most of the antiatoms thus created are untrapped and annihilate on the trap wall. Only the lowest energy subset of the antiatoms are trapped. Consequently, the temperature distribution of the trapped antiatoms scales as a truncated Maxwellian, i.e. as \( E \), where \( E \) is the antiatom energy. This distribution is, in the end, independent of the positron temperature, and we use it to initialize the energy of the antiatoms in our simulations. Rather than pick a specific upper truncation energy, we initialize the simulations with energies up to an energy generously beyond the our trapping well depth. Most of the antiatoms with energy above the trapping depth escape quickly, but simulations find that a few 'quasi-bound' antiatoms are slow to find an energetically-allowed escape 'hole', and remain trapped for substantial periods of time \([21, 22]\). Some aspects of this choice of distribution have been validated by comparing simulation and experimental results \([3, 18, 22, 23]\).

A typical simulated antiatom trajectory is plotted in figure 2. Although the motion in the \( z \) direction looks very sinusoidal in the short snippet shown in the figure, the oscillation frequency in a single trajectory often exhibits large variations over the long-term (see figure 3).

### 3. Chaotic nature of the trajectories

Visually, the long-term antiatom trajectories appear chaotic \([16, 18, 24]\). However, it had not been formally established that the trajectories in our system are truly chaotic. We explore this question by calculating the largest Lyapunov exponent (LLE) \([25]\) for the trajectories in our system; if the LLEs are positive in a bounded system like ours, then the system is chaotic.

In figure 4, we plot the numerically computed LLE \([26]\) for a large sample of 100 s trajectories. The average LLE is \( 178 \pm 97 \ \text{s}^{-1} \); only 4% have LLE less than 10 s\(^{-1}\) and might be compatible with zero. Thus, we conclude that the system is indeed chaotic. As a check, we also calculated the LLE for the non-chaotic harmonic oscillator system in which the potential is proportional to \( |x|^2 \) and whose depth is equal to the depth of our minimum-B trap. For this system, the average LLE is \( (1.9 \pm 2.4) \times 10^{-4} \ \text{s}^{-1} \), which, as expected, is consistent with zero.

Figure 5 shows the local exponential divergence \( \Gamma \) of nearby trajectories found by solving the local linearized force equation (see appendix B). Divergence occurs in two regions, the first being near the location of the mirrors. Here, the radial components of the mirror coil fields interact with the radial field of the octupole, producing azimuthally asymmetric \( B \) fields. Along with the asymmetries from the octupole ends, these asymmetries induce divergent trajectories which lead to chaos. Somewhat more surprising is the presence of...
divergence at smaller $z$ near $r = \sqrt{x^2 + y^2} = 0$. Here, the source of the divergence is the slight weakening of the $B_z$ fields from the mirror away from $r = 0$. This causes the absolute minimum of $|B(x)|$ to be at $r \approx 3$ mm, not $r = 0$; the $r$-axis is actually a slight local maximum. The true maximum is, of course, at large $r$ at the trap wall. The resulting low-domed ‘Mexican hat’ radial potential, in conjunction with coupling from the $z$-dependent terms, is likely the source of chaos for the trajectories that do not closely approach the mirrors.

4. Axial energy calculations

To explore the mixing between $E_1$ and $E_2$, we must be able to continuously determine these components of the conserved total energy $E$ from the trajectory in $(x, p)$. This is nontrivial, because the system Hamiltonian, equation (2), does not split into purely parallel and transverse components. However, the system potential $U(x)$ is concave-up and approximately symmetric around the $z = 0$ midplane [16]. Consequently $U(x = x_0, y = y_0, z)$ has an approximate minimum at the midplane for all $(x_0, y_0)$ in the trap. We have performed detailed calculations that include the current leads at the end of the octupole and interactions between the radially-directed fields of the mirrors and the octupole. These calculations show that the difference $U(x_0, y_0, 0) - U(x_0, y_0, z_{min})$ between the potential energy at $z = 0$ and the potential energy at the true minimum $z_{min}$, normalized to the trap well depth, is no

\[ \text{Figure 3. Ten second snippets of the axial bounce frequency of the trajectory shown in figure 2, showing that, unlike in the much shorter snippet in figure 2, the long-term behavior is irregular.} \]

\[ \text{Figure 4. Approximate largest Lyapunov exponent (LLE) values for 3149 trajectories versus each trajectory’s total energy $E$. The dashed red line corresponds to LLE = 0; chaotic trajectories will have a positive LLE.} \]
more than 0.3%. This maximum difference occurs at the trap wall; averaged over the entire midplane, this difference is 0.04%, and we will henceforth assume \( zm = 0 \).

Under the assumption that the potential energy at \( z = 0 \) is a minimum, we may assign all the potential energy at the midplane to the perpendicular direction, i.e. set \( U_{xy, z=0} = \mu \)\(^2\). Hence, the midplane parallel energy is entirely kinetic, and we can split the midplane energy into:

\[
E_p = \frac{p_r^2}{2M} + \frac{p_\perp^2}{2M} + U_{xy, z=0},
\]

where \( U_{xy, z=0} = \mu B(\mathbf{x}) \). The parallel kinetic energy is easy to compute from the simulated trajectories, though, given the finite step size used by our symplectic stepper, we do have to use quadratic interpolation to determine \( E_p \) at precisely \( z = 0 \). The total energy \( E \) is likewise easy to compute by summing equations (4) and (5). Since \( E \) is conserved, it need only be calculated once for a given trajectory.

Since \( E_p \) typically changes slowly on the time scale of the midplane crossings, it is sufficient, for the purposes of this paper, to monitor \( E_p \) at the midplane only. The \( z \) oscillation frequency is not constant within a trajectory, so the monitored axial energies form a nearly-periodic time-series:

\[
\{ (t_{ij}, E_{ij}) | i \in \mathcal{N}_j \},
\]

where \( t_{ij} \) is the time of the \( i \)th midplane crossing for the \( j \)th trajectory, \( E_{ij} \) is the axial energy at time \( t_{ij} \), and \( \mathcal{N}_j \) is the number of crossings for this trajectory. In figure 6, we show six representative samples of the normalized parallel energy time-series \( \varepsilon_{ij} = E_{ij}/E_j \), where \( E_j \) is the total energy for trajectory \( j \).

5. Trajectory stationarity

Figure 7(a) shows a typical scatter plot of the instantaneous values of \( (E, \varepsilon) \) at 1 s. The trajectories fill the available parameter space. Although individual trajectories change character dramatically with time, this scatter plot and other statistical properties of the ensemble of trajectories exhibit only small variations with time. For example, figure 7(b) shows that the cumulative distribution functions (CDFs) of the \( \varepsilon_{ij} \) distribution do not vary much between 1 and 1000 s.

6. Energy mixing time

In figure 8, we plot the average evolution of the deviations of \( \varepsilon_{ij} \). More precisely, for \( j = 1 \) to 51 541 trajectories, we plot

\[
\langle \sigma(t; T) \rangle = \left[ \frac{1}{N} \sum_{j=1}^{N} [\varepsilon_{ij}(t) - \varepsilon_{ij}(T)]^2 \right]^{1/2},
\]
the ensemble-averaged standard deviation of the difference between \( \Delta_{ij} \) at time \( t \) and at some earlier, fixed time \( \bar{t} \). Since energy \( E_j \) is conserved, any change in \( \Delta_{ij}(\bar{t}) \) must be accompanied by an equal and opposite change in \( \Delta_{ij}(t) = E_j(t)/E_i \).

**Figure 6.** Normalized axial energy \( e_{ij} \) versus time for a selection of trajectories. The total energies \( E \) are: (a) 0.079 K, (b) 0.147 K, (c) 0.315 K, (d) 0.391 K, (e) 0.477 K, and (f) 0.489 K. As described in section 9, the green dot is the initial parallel energy \( \epsilon_{ij}(\bar{t}) \) in our thresholding analysis for trajectory \( j \), the green dashed lines are the threshold lines, and the green hollow square indicate when the \( \epsilon_{ij} \) cross the threshold at time \( \bar{t}_j \). For some trajectories, like (b) and (e), the threshold lines are never crossed.

**Figure 7.** (a) Scatter plot of \( (E_j, \Delta_{ij}) \) for 3757 antiatom trajectories, evaluated at \( \bar{t} = 1 \) s. (b) CDFs of the \( \Delta_{ij}(\bar{t}) \) distributions of 37 577 antiatom trajectories at \( \bar{t} = 1, 10, 100 \) and 1000 s.
We find that $\langle \sigma(t; \bar{t}) \rangle$ increases quickly in the first tens of seconds; thus, the parallel and perpendicular energies must mix rapidly for at least some of the trajectories. As is more obvious in the figure 8 inset, the deviation approaches $\sim 0.26$ past 100 s, suggesting that the mixing time scale is generally less than 100 s for those particles that do mix. (Note that deviation may eventually exceed 0.26 for simulations that run longer than the 1000 s used for these simulations.) The similarity between the three plotted $\bar{t}$ curves again suggests that there is no gross evolution of the properties of the trajectories, though there is slight rearrangement between the $\bar{t} = 1$ and 100 s curves. As no significant differences are visible between the $\bar{t} = 100$ and 600 s curves, the rearrangement appears to be over by about 100 s.

### 7. Average axial energy

To better understand the behavior of individual trajectories, we plot, in figure 9, the time-average axial energy $\langle E_j \rangle \equiv \langle E_j \rangle = \frac{1}{\langle t_{j_{max}} \rangle} \sum_{j=1}^{N_{j_{max}}} E_{j_{max}} \Delta t_{ij}$, where $\Delta t_{ij} = t_i - t_{i-1}$ is the time between midplane crossings, for $j = 1$ to 3757 trajectories against the total energy $E_j$. Each trajectory was propagated for 1000 s. (Here, we use $\langle \rangle$ to indicate a time-average over a single trajectory, while $\langle \rangle$ indicates an ensemble average over all trajectories.)

In figure 9, there appear to be two categories of trajectories, one (`mix') with normalized averaged axial energy $\langle \varepsilon_j \rangle \approx 1/2$ ($\sim 66\%$ of the total number of trajectories), and the other (`no-mix') with normalized averaged axial energy $\langle \varepsilon_j \rangle \lesssim 1/10$ ($\sim 34\%$ of the total number of trajectories).

There is no evidence of clustering near $\varepsilon_j \approx 1/2$ in the figure 7(a) time snapshot. Thus, antiatoms in the mix category must be thoroughly mixing parallel and perpendicular energy as time advances to achieve an average of
Examples of such trajectories are shown in figures 6(a), (c), (d), (f), though some trajectories, like the one shown in figures 6(c), (f), exhibit behaviors of both categories. Antiatoms in the no-mix category do not exchange significant parallel and perpendicular energy, as evidenced by the parallel energy remaining a small fraction of the total energy. Examples of such trajectories are plotted in figures 6(b), (e). Nonetheless, since we found few non-chaotic trajectories in our LLE analysis, these trajectories are chaotic. The boundary between the mix and no-mix categories is somewhat arbitrary; in figure 9 we plot the boundary used in the remainder of this paper. Other simulations show that about 3% of the trajectories change category in 500 s.

One might think that the proportionality between $E_{|| \perp}$ and $E_{||}$ for the mix trajectories should be $1/3$, not $1/2$. However, the confining potential for the antiatoms resembles a brick wall in $r$ because the octupole field, which scales as $r^3$, adds in quadrature to the solenoidal field when calculating the magnetic field magnitude; only $|B|$ enters the potential. Thus, the potential increases like $r^6$ for small $r$, trending towards $r^3$ for large $r$. As a consequence, the potential energy’s dependance on the transverse coordinates is relatively unimportant, and the total energy has only four effective degrees of freedom. Further, though $E_{|| \perp}$ is set to the kinetic energy at the midplane, it has there momentarily absorbed all the parallel potential energy. This suggests that the average $E_{||}$ should be half the total energy $E$ as it sums two of the four degrees of freedom, regardless of whether the average is taken over time for a single trajectory or over the ensemble of trajectories at a single time.

8. Equilibrium axial energy

Antiatoms on mix orbits are initialized with a wide range of $E_{||}$ at $t = 0$. Notwithstanding the arguments in the previous section, it is curious that all these atoms possess time-averaged $\langle E_{||} \rangle$ in a fairly narrow band around $1/2$. This is especially true as the initial velocities are isotropic, which sets $\langle E_{||} \rangle = 1/3$ when the antiatoms are launched at $t = 0$. In figure 10 we investigate this issue. The figure shows the ensemble-averaged $\langle E_{||} \rangle$ as a function of time for three cuts of the data: trajectories that mix, trajectories that do not mix, and the ensemble of all trajectories. As expected from the data in figure 9, $\langle E_{||} \rangle$ for the mix trajectories is nearly $1/2$. More precisely, $\langle E_{||} \rangle$ for the mix trajectories approaches 0.485 from an initial value at $t = 0$ of about 0.472. The no-mix trajectories have an average $\langle E_{||} \rangle$ of 0.043. The entire ensemble has an average $\langle E_{||} \rangle$ of 0.348. This latter is in accord with the value of $\langle E_{||} \rangle = 1/3$ at $t = 0$. Thus, it could be that $\langle E_{||} \rangle \approx 1/2$ for the mix trajectories is simply an initial condition artifact of the mix cut.
To determine if $1/2$ is indeed an initial condition artifact or if the dynamics converge towards this value for the average $\langle \epsilon_i \rangle$ for the mix trajectories, we modeled trajectories on which we deliberately kicked $v_f$ at $t = 400$ s. We used two strengths of kicks, and both increased and decreased $v_f$. The effects on $\langle \epsilon_i(t) \rangle$ are also shown in figure 10. For the mix trajectories, $\langle \epsilon_i(t) \rangle$ relaxed back to $\sim 1/2$ on a time scale on the order of 100 s, establishing that this is indeed a special value of $\langle \epsilon_i \rangle$, not an artifact of the initial conditions. Note that the increase and decrease trajectories are averaged over a specific subset of the data: trajectories that were in the mix category before the kick, and remained in the mix category after the kick.

For runs in which the kick increased $\langle \epsilon_i \rangle$, the kick was sufficient to cause some (23% and 14%, for the strong and weak kicks, respectively) trajectories to intersect the trap wall. Further, the kicks were sufficient to 'promote' some trajectories from the no-mix category before the kick into the mix category after the kick. These promote trajectories, which constituted 22% and 15% of the no-mix trajectories, are separately plotted in figure 10, and also relax to $\langle \epsilon_i \rangle \approx 1/2$, albeit on a slower time scale than for the trajectories which were in the mix category before the kick.

For the no-mix trajectories, there was, as expected, no tendency to relax immediately after the kick, though for the large increase kick, some of the trajectories begin to change into the mix category at late times. The decrease kick was strong enough to 'demote' some (22% and 8%) of the trajectories from the mix category into the no-mix category; these demoted trajectories also show no large relaxation post-kick.

9. Quantifying the energy mixing time

The data in figures 8 and 10 suggest an energy mixing time of the order of 100 s, but do not straightforwardly yield the distribution of these times for different trajectories. Figure 6 suggests that there are wide variations in the mixing times; qualitatively, these times vary between a few tenths of seconds to at least two thousand seconds. We use a thresholding method to quantitatively determine the mixing time distribution. Many more common and perhaps more powerful methods of determining the mixing time, like autocorrelation computations, are complicated by the aperiodic nature of the $t_{fp}$.

For every trajectory $j$, the thresholding procedure begins by selecting an initial parallel energy value $\epsilon_{ij}$, where the index $k$ is randomly selected so that $t_{ik}$ is between 1 and 2 s. This $k$ interval is chosen to be after any initial transients, but before significant computational resources have been expended. The selected initial ($t_{kij}, \epsilon_{ij}$) are indicated by the green circles in figure 6. Next, we compute thresholds $\epsilon_{ij} \pm \epsilon_{ij}$; Thresholds of $\epsilon_{ij} = 0.2$ are plotted as the green lines in figure 6; in some cases, the threshold lines fall outside the allowed range $\{0, 1\}$ for $\epsilon_{ij}$, and are not plotted. Next, we find the index $l$ and corresponding time $t_l$ for which $\epsilon_{il} \pm \epsilon_{ij}$ first traverses a threshold, as indicated by the green hollow squares in figure 6, and record the tuple $(E_j, \epsilon_{ij}, t_l)$, where the time to cross the threshold is $t_l = t_b - t_f$. For computational efficiency, we also terminate propagating the trajectory at $t_f$.

We recognize that the threshold crossing-time $t_l$ does not incorporate all the information in a given trajectory. Indeed, it sometimes appears to be a mismeasure; for instance, it appears to be too short for the $\epsilon_{ij}$ trajectory, and too long for the $\epsilon_{ij}$ trajectory. Further, sometimes the threshold is never crossed. In these cases, we arbitrarily cut off the simulation at $t_{cut} = 2000$ s and set $t_{lj}$ to this time. Nonetheless, we believe that by studying a sufficiently large sample of trajectories, we can obtain reliable estimates of the energy mixing time.

10. Mixing time results

We compiled $(E_j, \epsilon_{ij}, t_{lj})$ tuples for $\sim 40,000$ trajectories. (Quasi-bound antiatoms that escaped before reaching a threshold were discarded.) In figure 11(a), we plot the CDF of the crossing-time distribution $t_l$ for various thresholds $\epsilon_{ij}$ in the range of $\{0.005, 0.5\}$. Note that the axial bounce times are on the order of 10 ms so our $\epsilon_{ij}$ diagnostic loses accuracy for $t_l$ near this boundary. Further, uninteresting boundary effects arise when $\epsilon_{ij} \gtrsim 0.5$; if the initial value of $\epsilon_{ij} \approx 0.5$, the threshold lines $\epsilon_{ij} \pm \epsilon_{ij}$ could both be outside of the allowed range $\{0, 1\}$.

For thresholds with $\epsilon_{ij} \gtrsim 0.2$, the data in figure 11(a) indicates that about 65% of the trajectories mix in 2000 s. These trajectories are in the mix category identified earlier. For smaller thresholds $\epsilon_{ij} \leq 0.01$, the data shows that nearly all the trajectories mix. Thus, many trajectories in the no-mix category actually do experience at least some mixing, albeit mixing involving a very small fraction of the available total energy. (Note that simulation time step studies suggest that the computational errors in figure 11(a) are well less than 1%.)

Low level mixing is quite fast. For the $\epsilon_{ij} = 0.005$ threshold in figure 11(a), for example, over 50% of the trajectories mix in $\sim 10$ ms. This time scale is compatible with the calculated values of the LLE $\sim 100$ s$^{-1}$ in figure 4.
The intersections of the curves in figure 11(a) with a horizontal line yield information about the time it takes to reach the listed thresholds. Thus, for the CDF $= 0.3$ line for example, we can interpret the $t_\beta$ at the intersections to be the time that it takes 30% of the trajectories to make an excursion equal to the associated $e_\beta$ at each intersection. In figure 11(b), we plot the excursions $e_\beta$ thus attained as a function of time $t_\beta$ for various values of the CDFs in (a). As expected from a random walk process, the $e_\beta$ increase in proportion to $t_\beta$, at least over a substantial range. Thus, large excursions can take significantly longer than the times predicted directly from the LLE.

We have chosen the threshold $e_\parallel = 0.2$ for our remaining studies. Obviously the choice of a single $e_\parallel$ to characterize the mixing time is somewhat arbitrary, but this value requires a substantial change in $e_\parallel$, while generally remaining far from boundary effects. Using this threshold, we find that mixing occurs quickly along many of the trajectories, but a substantial fraction do not mix in under 2000 s. Specifically, with $e_\parallel = 0.2$, 25% mix within 1.3 s, 50% mix within 19 s, and 60% mix within 120 s, but 34% do not mix in under 2000 s. Figure 12(a) shows that the mixing times are similar for all but the trajectories with the lowest and highest total energies $E$. However, as shown in figure 12(b), the dependence on $e_\parallel$ is stronger; by 10 s, 80% of the antiatoms with $0.4 > e_\parallel > 0.2$ mix.

To obtain a more granular understanding of the mixing times, in figure 13 we bin the reduced tuples $(E_j, \epsilon_{\parallel/k})$ into $10 \times 20 = 200$ bins of increments $\Delta E = 0.05$ K, $\Delta \epsilon_{\parallel} = 0.05$, and indexed by $m$ and $n$. We then considered the distribution function of the $t_\parallel$ in each bin. Examples of these distributions are plotted in figure 13. Generally, the distributions can be fit with an exponential function characterized by an average threshold crossing-time of $t_\parallel$, estimated from a maximum likelihood calculation. This calculation is complicated by the 34% of trajectories that never cross their energy threshold. The methodology we use is given in the appendix C (see, in particular, equation (C.4)).

The results of calculating $t_\parallel$ for each of the 200 bins in figure 13 are plotted in figure 14. As expected, there is a wide variation—at least four orders of magnitude—of the threshold crossing times, and hence of the energy mixing times. The variation is primarily correlated with the normalized parallel energy, and secondarily with the total energy.
11. Error fields, variant magnetic systems and trajectory initiation

All the studies reported in this paper to this point were performed in a simple magnetic system with two distant mirrors and an octupole. This is the magnetic system used in the original antiatom trapping, spin flip, gravity,
and charge experiments [1–4]. In this section we consider the effect of magnetic errors, variant magnetic systems, and initial distributions.

11.1. Error fields
Despite careful construction, any magnetic system will inevitably contain errors. For example, the ALPHA external solenoid is not precisely fixed with respect to the magnetic trap, and $B_{\text{solv}}$ could be tilted with respect to the trap axis. This tilt is less than 2 mrad in the ALPHA system [23]. Figure 15(a) shows that such tilts increase the mixing fraction, but that the effect is small. As another representative magnetic error, we considered quadrupolar contamination of our desired octupolar field. While we have not measured the size of this error on ALPHA, we believe that the quadrupolar component of the field is less than 1% of the octupolar component at the trap wall. Figure 15(b) shows that the effect of such contamination is also small. Though the two tests reported in figure 15 are not exhaustive, they suggest that the results of this paper are robust against magnetic field errors.

11.2. Axial flatness variants
By energizing the three interior mirrors in addition to the two most distant mirrors, we can adjust the flatness of the magnetic field $|B|$ as a function of the axial position $z$. In figure 16, we compare two magnetic configurations with different axial flatnesses to our standard configuration. Mixing is much more rapid when the field is far from flat, and the trajectories are confined to a small central region. For this ‘tight’ configuration, the no-mix category of trajectories vanishes. That the mixing would be more rapid is expected, as the strong axial magnetic gradients generate proportionally large radial components to the mirror fields. As noted in the discussion of figure 5, these radial fields will interact with the radial fields of the octupole, resulting in large azimuthal asymmetries which can easily mix parallel and perpendicular energies. The mixing times in the ‘flat’ trap, which is similar to the trap used for 1S-2S [5] and hyperfine [6] spectral measurements, is somewhat faster than in the normal trap, likely because the energized interior mirrors cause mixing.

11.3. Trajectory initiation
The CDFs plotted in figures 12, 15, and 16 depend on the characteristics of the trajectories present in the simulations. A different initiation of the trajectories could result in a different distribution of these characteristics, and thus a different CDF. In our standard simulations, we assume that the antiatoms are born in the ground state ($n = 1$). This is unlikely to be correct; we believe that the antiatoms are born in high $n$ states, perhaps $n = 40$, and cascade down the ground state over a period of less than one second. This cascade cools the antiatoms [27, 28], and could change the trajectory characteristics. The cascade is easy to simulate [29]. (As yet, no experimental measurements prove that the cascade initiation better models the experiments.) The results of simulations with the cascade initiation are shown in figure 16, and are not interestingly differently from the results with ground state initiation.

Figure 14. Values of characteristic mixing time $t_\beta$ for the bins in figure 13. The contour lines were generated using a cubic b-spline algorithm. The markers (a), (b), and (c) correspond to the labeled bins in figure 13.
Figure 15. (a) Effect of a tilt error on the CDFs of the $t_{ij}$. The heavy solid red curves is the standard magnetic configuration, while the other curves show the CDF for the indicated solenoidal tilts. (b) The CDF of the $t_{ij}$ of the system with a quadrupolar contribution added to the octupole field. The heavy solid red curve is again the CDF of the standard magnetic configuration, while the other curves show the CDF with quadrupolar components at the trap wall of the indicated fraction of the octupole field.

Figure 16. Effect of different field configurations on the CDF of the $t_{ij}$ as a function of time. The on-axis field profiles for three mirror configurations are shown below the graph. One configuration substitutes a quadrupole magnet for the octupole. CDFs for the standard trajectory initiation (see text) are plotted as solid lines; CDFs for trajectories with cascade initiation are shown as dashed lines.
11.4. Quadrupole
All the studies reported in this paper to this point were undertaken with an octupole magnet. Reference [16] predicted that trajectories in a quadrupole experience little mixing compared to those in an octupole. We confirm this prediction here. For a quadrupole, the average LLE is $14 \pm 16 \text{ s}^{-1}$, much lower than in an octupole, and possibly compatible with zero. In simulations of $\sim 13$ 000 trajectories, only 465 (3%) crossed the $\pm e_{1}^{1} = 0.2$ energy mixing thresholds in less than 1000 s (see figure 16). Thus, the energy mixing time in a quadrupole is orders of magnitude longer than in an octupole.

12. Conclusions

In this paper, we used computer simulations to analyze the characteristics of antiatom trajectories in an octupole-based minimum-B trap; the dynamics show surprising richness. We have established that almost all of the trajectories are chaotic. For approximately two thirds of the trajectories, the antiatoms mix their parallel and perpendicular energy; roughly half substantially exchange these energies in less than ten seconds. The remaining third of the trajectories do not mix these energies in less than one thousand seconds. The trajectories can be classified into these two categories by their ratio of parallel to perpendicular energy: those trajectories with ratios below approximately 0.1 fall into the no-mix category.

Our observations help us understand and optimize experimental protocols for precision measurements on antihydrogen. For example, we can expand the trap size axially by manipulating the mirror currents. If we do this quickly, but adiabatically, the resulting adiabatic expansion cooling will cool the antiatoms in the parallel $\hat{z}$ direction only. This will move the ensemble of parallel energies towards low $\hat{y}$ i.e. towards the non-mixing category. This is advantageous for planned gravity experiments [3, 16, 30, 31], which intend to balance the parallel directed energy with a magnetic gradient. Mixing between the parallel and perpendicular energies upsets this balance and confounds the intended measurements by causing untimely antiatom escapes from the trap.

Similarly, such fast adiabatic expansion cooling is beneficial for Lyman-alpha laser interaction studies. Only cooling in the parallel direction is necessary to reduce the doppler width of the measurement. However, for the 1S-2S line, the dominant error is transit time broadening [32], which can only be reduced by cooling the perpendicular energy. Adiabatic expansion cooling that only cools the parallel direction is not beneficial, and the expansion process would have to be done in such a fashion that the parallel and perpendicular energies stay in contact. Likewise, laser cooling, which would largely cool only the parallel direction in the geometry of the ALPHA experiment [17], is less effective than if it would be if the parallel and perpendicular energies would mix quickly.

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Appendix A. Magnetic field model

The model we use to describe our fields is given in detail in [18]; here we present a summary. In cylindrical coordinates, we approximate the field from the mirror coils as

$$A_{\phi} = C \frac{1}{2a\lambda} [(a^2 + R^2 - 2a\lambda r)^{-1/2} - (a^2 + R^2 + 2a\lambda r)^{-1/2}], \tag{A.1}$$

where $A_{\phi}$ is the azimuthal component of the vector magnetic potential, $C = I\mu_{0}a^2/4$ is a constant proportional to the mirror current $I$, $a$ is the radius of the mirror, $R^2 = r^2 + z^2$ with $x, y, z$ measured from the center of the mirror, and $\lambda$ is a dimensionless fit parameter. With $\lambda = \sqrt{3}/2 \approx 0.866$, equation (A.1) exactly reproduces the first two terms of the exact $A_{\phi}$ for a loop of current [33]. We adjust $a$ and $\lambda$ to best fit the field from our finite size mirror coils as determined by an accurate, but slow, Biot–Savart calculation.

The vector potential for an infinite octupole is $A_{\infty} = Fr^4 \cos(4\phi)\hat{z}$, where $F$ is a constant. A finite, symmetric octupole can be written as

$$A_{z} = [F_{r}(r) r^4 + F_{k}(z) r^k + F_{b}(z) r^b + ...] \cos(4\phi), \tag{A.2}$$
where the $F$'s are functions which can all be related to $F_2(z)$ by requiring that $\nabla^2 A_z = 0$. We choose
\[ F_2(z) = \Delta \sigma \frac{1}{\Delta z} \left( \text{erfc}(z), \frac{1}{\Delta z} \right) - \text{erfc}(z), \frac{1}{\Delta z} \right), \tag{A.3} \]
where $D$ is a constant, $\Delta z$ is the approximate ends of the octupole and $\Delta z$ is the distance in $z$ over which the octupole drops to near zero. Again, we fit these parameters to the field calculate by Biot–Savart.

The solenoidal field in our experiment is simply a constant field pointing in $\hat{z}$. The sum of the mirror, octupole, and solenoidal field is accurate to about 1% over the region of the magnetic system accessible to the antiatoms.

**Appendix B. Local exponential divergence**

From equation (2) the system force equation can be written as
\[ \dot{M} = -\mu_0 \nabla |B(x)|. \tag{B.1} \]

For any trajectory passing through $(x_0, y_0, z_0, v_{x0}, v_{y0}, v_{z0})$, we can solve for the perturbed trajectory passing through $(x_0 + \Delta x, y_0 + \Delta y, z_0 + \Delta z, v_{x0} + \Delta v_{x0}, v_{y0} + \Delta v_{y0}, v_{z0} + \Delta v_{z0})$ in the system linearized around $(x_0, y_0, z_0)$. Defining $\Delta x = (\Delta x, \Delta y, \Delta z, \Delta v_{x0}, \Delta v_{y0}, \Delta v_{z0})$, then
\[ d\Delta x/dt = A\Delta x, \tag{B.2} \]

where
\[ A = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -(\mu_0/M)|B|_{xx} & -(\mu_0/M)|B|_{xy} & -(\mu_0/M)|B|_{xz} & 0 & 0 & 0 \\ -(\mu_0/M)|B|_{yx} & -(\mu_0/M)|B|_{yy} & -(\mu_0/M)|B|_{yz} & 0 & 0 & 0 \\ -(\mu_0/M)|B|_{zx} & -(\mu_0/M)|B|_{zy} & -(\mu_0/M)|B|_{zz} & 0 & 0 & 0 \end{pmatrix} \tag{B.3} \]

and where $|B|_{ij} = \partial^2 |B(x)|/\partial y \partial x$, etc. Then, the local exponential divergence $\Gamma$ used in section 3 is the largest real part of the eigenvalues of $A$.

**Appendix C. Likelihood maximization for $\tau_j$**

Consider $p$ samples with $t_{ij} \leq t_{cut}$, and $q$ samples with $t_{ij} > t_{cut}$, pulled from an exponential distribution $P(t_{ij}; \tau_j) = (1/\tau_j) \exp(-t_{ij}/\tau_j)$ with characteristic time $\tau_j$. For these samples, the log-likelihood function for $\tau_j$ is
\[ \log [L(\tau_j | t_{ij})] = \log \left[ \left( \prod_{j=1}^{p} P(t_{ij}; \tau_j) \right) \times \left( \prod_{j=1}^{q} P_j \right) \right], \tag{C.1} \]

where $P_j = \int_{t_{cut}}^{\infty} P(t_{ij}; \tau_j) \, dt_j = \exp(-t_{cut}/\tau_j)$ is the probability that $t_{ij} > t_{cut}$. Then:
\[ \log [L(\tau_j | t_{ij})] = \log \left[ \left( \prod_{j=1}^{p} \frac{1}{\tau_j} e^{-t_{ij}/\tau_j} \right) \times \left( \prod_{j=1}^{q} e^{-t_{cut}/\tau_j} \right) \right] \tag{C.2} \]
\[ = p \log \frac{1}{\tau_j} - \frac{p}{\tau_j} \frac{\sum_{j=1}^{p} t_{ij}}{\tau_j} - q \frac{t_{cut}}{\tau_j}. \tag{C.3} \]

Maximizing the log-likelihood by setting the derivative of equation (C.3) to zero yields the best estimate for $\tau_j$, namely:
\[ \tau_j = \frac{\sum_{j=1}^{p} t_{ij}}{p} + q t_{cut}. \tag{C.4} \]

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