Fundamental Limit to Atom-Ion Sympathetic Cooling in Paul Traps

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We present a fundamental limit to the sympathetic cooling of ions in radio-frequency traps using cold atoms. The limit arises from the work done by the trap electric field during a long-range ion-atom collision and applies even to cooling by a zero-temperature atomic gas in a perfectly dc-compensated trap. We conclude that in current experimental implementations this collisional heating prevents access to the quantum regimes of atom-ion interaction or ion motion. We determine conditions on the atom-ion mass ratio and on the trap parameters for reaching the s-wave collision regime and the trap ground state.

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The combination of cold trapped ions and atoms [1–6] constitutes an emerging field that offers interesting and hitherto unexplored possibilities for the study of quantum gases. New proposed phenomena and tools include sympathetic cooling to ultracold temperatures [7, 8], charge transport in an atomic gas [9], dressed ion-atom states [10–13], local high-resolution probes [14, 15] and ion-atom quantum gates [16, 17].

In contrast to atom traps that are based on conservative forces, radiofrequency ion traps (Paul traps) employ time-varying electric fields to create a time-averaged secular trapping potential [18]. The time-varying field can pump energy into the system if the ion's driven motion is disturbed, which raises the question to what extent the ion can collisionally thermalize with a cold atomic gas that it is embedded in. Four decades ago, Major and Dehmelt analyzed this problem by approximating the ion-atom interaction as a hard-core potential, and concluded that sympathetic cooling is possible as long as the ion-to-atom mass ratio exceeds unity [19]. However, as we show below, a more refined analysis that includes the attractive long-range r^{-4} atom-ion potential leads at low temperatures to a different conclusion.

Paul traps employ a spatially varying radiofrequency (RF) electric field that drives a micromotion at the RF frequency with an amplitude proportional to the local field. At any position and time, the ion's velocity can be decomposed into the micromotion velocity and the remaining velocity of the secular motion. To understand the sympathetic cooling and heating processes described by Ref. [19] in an intuitive physical picture, consider the simple case of a sudden collision with an atom that brings an ion to rest, a process which in a conservative trap would remove all kinetic energy. Immediately after such a collision the ion's secular velocity is equal and opposite to the micromotion velocity at the time of the collision. This secular velocity can be larger or smaller than before the collision. In particular, if at the time just preceding the collision the ion's micromotion velocity exceeded the secular velocity, the ion's secular energy will be increased, i.e., the ion will be heated even in a collision that brings it momentarily to rest. This picture also makes it clear that if a trap is not dc-compensated, i.e. if a dc electric field displaces the trap minimum from the node of the RF field, then the average RF-induced collisional heating will be larger due to the increased micromotion [20]. Currently realized ion-atom systems are limited by incomplete compensation of the dc field, with the lowest directly observed equilibrium ion temperature being on the order of 1 K [3]. Quantum effects in these systems, on the other hand, are characterized by the much smaller temperature scales $\hbar\omega/k_B \sim 50\mu$K for the trap zero point motion and $E_s/k_B \sim 50$ nK for the s-wave collision threshold [21].

In this Letter, we show that even in a perfectly dc-compensated Paul trap, a fundamental limit to sympathetic atom-ion cooling arises from the electric field of the atom when polarized by the ion, or equivalently, the long-range ion-atom interaction. The displacement of the ion from the RF node by the approaching atom leads to micromotion, whose interruption causes heating. A second nonconservative process arises from the non-adiabatic motion of the ion relative to the RF field due to the long-range atom-ion potential; during this time, the trap can do work on the ion and increase its total energy.

We show that, in realistic traps, the work done by the RF field dominates the effect of the sudden interruption of the ion's micromotion and leads to an equilibrium energy scale that, for all but the lightest atoms and heaviest ions, substantially exceeds both the s-wave threshold E_s and the trap vibration energy $\hbar\omega$. Our analysis shows that current atom-ion experiments [1–6] will be confined to the classical regime, and indicates how to choose particle masses and trap parameters in order to reach the quantum domain in future experiments.

Our analytical results are supported by numerical calculations that furthermore reveal that in those collisions where the RF field removes energy from the system, the atom becomes loosely bound to the ion, leading to multiple subsequent close-range collisions until enough energy is absorbed from the RF field to eject the atom and heat the ion. In a quantum picture, the latter process process can be thought of as the trap RF field exciting transitions between the closely spaced near-threshold states in the ion-atom potential.

We consider a classical model and later confirm that this assumption is self-consistent, i.e. that the equilibrium energies obtained from the model are consistent with a classical description. An atom of mass m_a approaches from infinity to an ion of mass m_i held stationary in the center of an RF quadrupole trap. At sufficiently low collision energies, the angular-momentum barrier will be located far from the collision point, and will not influence the collision dynamics once the barrier is passed. For simplicity, and for deriving the energy and length scales of the problem, we initially assume a one-dimensional (1D) collision in a quadrupole RF potential given by $V(r_i, r_a, t) = e\mathcal{E}(r_i, t)\, r_i/2 + U(r)$, where e is the ion's charge, r_i and r_a are the ion and atom locations, respectively, $r = r_i - r_a$ is the ion-atom distance, and $\mathcal{E}(r_i, t) = g r_i \cos(\Omega t + \phi)$ is the RF electric field of the ion trap at frequency Ω parameterized by its quadrupole strength g. The ion-atom interaction potential is given by $U(r) = -C_4/(2r^4)$ at large distances [21], and modeled as a hard-core repulsion at some small distance.

As the ion is pulled from the origin of the trap by the long-range interaction U with the approaching atom, the oscillating electric field $\mathcal{E}$ causes it to execute sinusoidal micromotion with amplitude $qr_i/2$ where $q = 2eg/(m_i\Omega^2)$ is the unitless trap Mathieu parameter (chosen in physical traps as $q < 0.5$ to ensure stability). As long as the motion of the ion relative to the atom remains slow in comparison to the RF frequency, the ion's equations of motion during one RF cycle will remain linear and the secular motion of the ion during each RF cycle can be described in terms of an effective conservative secular potential $V_s = \frac{1}{2}m_i\omega^2 r_i^2 + U(r)$, where $\omega \approx q\Omega/2^{3/2}$ is the vibration frequency of the ion trap. Associated with V_s are the characteristic length scale $R = \left(C_4/m_i\omega^2\right)^{1/6}$, time scale $T = 2\pi/\omega$, and energy scale $E_R = \frac{1}{2}m_i\omega^2R^2 = \frac{1}{2}(m_i^2\omega^4C_4)^{1/3}$ at which the interaction potential U is equal in magnitude to the trap harmonic potential.

In collisions with light atoms, $m_a < m_i$, we expect the ion to stay confined close to the trap origin; in this case, the dependence of the ion-atom distance r on time is governed solely by the motion of the atom in the ion-atom potential U as

$$r(t) \approx (9C_4/\mu)^{1/6}\, |t|^{1/3}, \tag{1}$$

where the collision occurs at time $t = 0$ and $\mu = m_i m_a/(m_i + m_a)$ is the reduced mass of the system. The displacement r_c of the ion from the center of the trap at the time when the hard-core collision with the atom occurs can then be estimated by integrating the effect of the force $2C_4/r^5$ exerted by the atom on the ion trapped in its secular potential, yielding $r_c \approx 1.11\,(m_a/m_i)^{5/6}\,R$. In collisions with heavy atoms ($m_i < m_a$) on the other hand, the ion responds quickly to minimize the total secular potential energy until, at $(r_i, r_a) = (0.29,\, 1.76)\,R$, the deformed ion's equilibrium position becomes unstable and the light ion quickly falls towards the atom with the collision occurring at $r_c \approx 1.76R$. In general, the collision point can be computed by numeric integration of the system's secular equations of motion which, when expressed in the (R, T, E_R) units, depend only on the ion/atom mass ratio m_i/m_a.

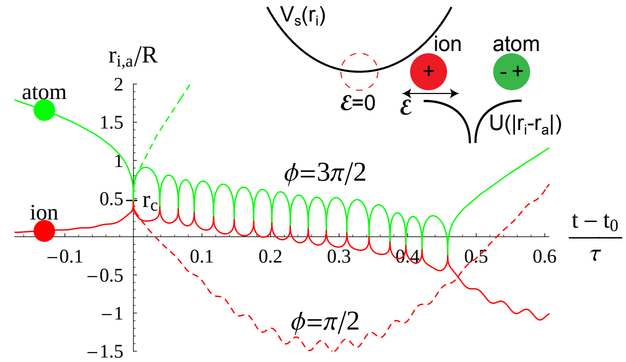

Figure 1: Trajectories of an ion $r_i(t)$ and an atom $r_a(t)$ during a classical one-dimensional low-energy collision. The atom of mass m_a approaches the ion of mass $m_i = 2m_a$ held in the center of a RF trap with secular frequency $\omega = 2\pi/\tau$ and Mathieu parameter $q = 0.1$, leading to a hard-core collision at $r_i = r_a = r_c$, $t = 0$ and RF phase ϕ. For $\phi = \pi/2$ (dotted lines), the trap field adds energy to the system, causing heating. For $\phi = 3\pi/2$ (solid lines), the RF field removes energy, binding the atom to the ion and causing further collisions at various RF phases until enough energy is accumulated to eject the atom.

As the RF field at the collision point r_c is nonzero, we may expect the hard-core collision with the atom to change the system energy on the scale of the ion's average micromotion energy at this point, $E_{\mu m} \approx m_i\omega^2 r_c^2/2$. In general, the energy of the system can change during the whole interval in which the ion is moving non-adiabatically relative to the RF field, including the interval $-t_1 < 0 < t_1$ around the collision at $t = 0$, during which the ion's velocity $\dot{r}_i$ is greater than its average micromotion velocity $v_{\mu m} \approx \omega r_c$. In this regime, the trap RF field can be thought of as a time-dependent perturbation to the ion-atom potential, doing work on the ion equal to

$$W = e\int_{-t_1}^{t_1} \mathcal{E}\left(r_i(t), t\right) \cdot \dot{r}_i(t)\, dt. \tag{2}$$

For $\dot{r}_i \gg v_{\mu m}$, we may neglect the effect of the electric field on the ion's trajectory and approximate the ion's

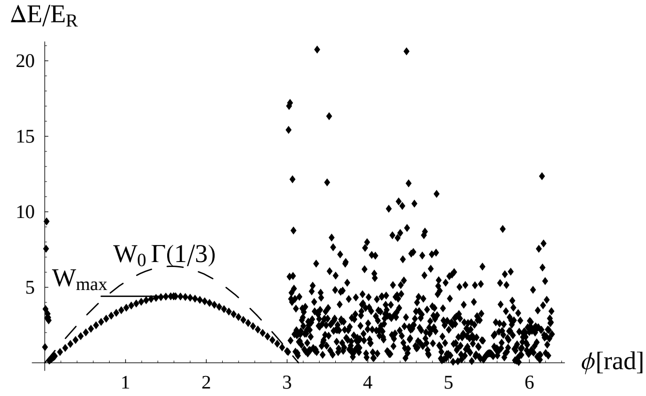

Figure 2: Change ΔE in the total secular energy of a colliding ion-atom system ($m_a/m_i = 1/2$, $q = 0.1$), as a function of the RF phase ϕ during the first hard-core collision. For $0 < \phi < \pi$, the system undergoes only one collision with energy gain comparable to the analytic prediction (3) (dashed line). For $\pi < \phi < 2\pi$, the atom is bound and undergoes several collisions with the ion before eventually escaping, leading to a sensitive dependence of the total energy gain ΔE on the initial conditions.

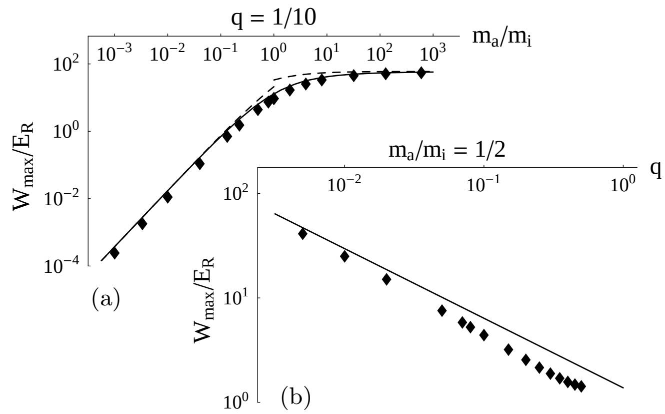

Figure 3: Maximal energy gain $W_{\max}$ in a low-energy 1D ion-atom collision as a function of the atom/ion mass ratio m_a/m_i with Mathieu parameter $q = 0.1$ (a) and as a function of q with $m_a/m_i = 1/2$ (b). Data points are numeric calculations. The solid line corresponds to $W_{\max} = \Gamma(1/3)\, W_0$ where the collision point r_c is calculated numerically using the secular potential approximation, and the dashed lines represent the light- and heavy-atom estimates ($r_c/R \approx 1.11\,(m_a/m_i)^{5/6}$ and $r_c/R \approx 1.76$, respectively).

position in terms of the free collision trajectory $r(t)$, Eq. 1, as $r_i \approx r_c - r(t)\, m_a/(m_i + m_a)$. The work done by the RF field can then be written as $W = W_{\max}\sin\phi$, where ϕ is the RF phase at the time of the hard-core collision. The maximal energy gain of the system after one collision $W_{\max}$ is approximated by

$$W_{\max} \;\approx\; W_0 \int_{-\Omega t_1}^{\Omega t_1} \mathrm{sgn}\tau\, |\tau|^{-2/3} \sin(\tau)\, d\tau \qquad (3)$$

with

$$W_0 = \frac{r_c}{R}\left(\frac{8m_a}{m_i + m_a}\right)^{5/6} (3q)^{-2/3}\, E_R \qquad (4)$$

the characteristic energy scale of the work done on the ion by the RF field expressed in terms of the energy scale E_R of the secular potential V_s. The non-adiabatic condition $|\dot{r}_i| > |v_{\mu m}|$ is equivalent to $3q\Omega t < (2R/r_c)^{3/2}(1 + m_i/m_a)^{-5/4}$, which, for the practically relevant values of $q < 0.5$, will always include the region $|\Omega t| < 0.8$ where the dominant contribution to the integral in (3) occurs. Consequently, we may extend the limits of integration to $\pm\infty$ to obtain $W_{\max} \approx \Gamma(1/3)\, W_0$ where $\Gamma(1/3) = 2.68$ is the Euler gamma function.

For $q < 0.5$, $W_0/E_{\mu m} > 2$, and the gradual energy change (2) dominates the effect of the sudden interruption of the ion's micromotion. Intuitively, as the collision energy is lowered, the ion-atom potential determines the dynamics at longer times, giving the RF field more time to do work on the system. Since the trap electric field must be increased at high RF frequencies in order to preserve the ion secular potential, the gradual heating also increases with a decrease in the Mathieu parameter.

Since W corresponds to the difference in the work done by the RF field during the incoming and outgoing parts of the collision, the energy change will depend on the phase ϕ of the RF field at the time of the hard-core collision. For $0 < \phi < \pi$, the RF field accelerates the collision partners towards each other and causes heating; for $\pi < \phi < 2\pi$, the RF field opposes the collision, doing negative work and causing the atom to be bound to the trapped ion with binding energy on the order of $-W_0$ (Figure 1). Since the r^{-4} potential does not possess stable orbits, bound ion-atom trajectories will include further close-range collisions. Depending on the RF phase during each such collision, the system will gain or lose energy on the order of W_0, leading to a random walk in energy space until the atom finally unbinds, leaving the system with a net energy gain also on the order of W_0 (Figure 2).

To quantitatively confirm the above heating model, we numerically calculated classical trajectories of 1D ion-atom collisions as function of the RF phase ϕ, the mass ratio m_a/m_i and the Mathieu parameter q (Figures 1, 2 and 3). The ion was initially held fixed at the center of the trap and the atom allowed to approach along the analytic trajectory (1). At an ion-atom distance r such that $C_4/(2r^4) \ll W_0$, the ion was displaced from the trap to balance the force exerted by the atom and the numeric integration started. The equations of motion were integrated using the Dormand-Prince explicit Runge-Kutta method: away from collision points, the motion was integrated as a function of time while near the collisions, the ion-atom distance r was used. The accuracy of integration was confirmed by replacing the RF potential with

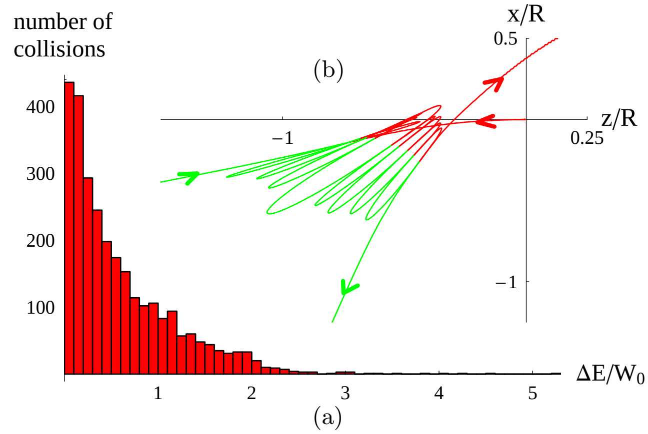

Figure 4: (a) Distribution of numerically computed secular energy gains in 2883 random low-energy collisions between a free ^{87}Rb atom and a ^{174}Yb$^+$ ion held in the three-dimensional trap from [2], in units of the micromotion heating energy scale W_0. A sample ion-atom collision trajectory is shown in the inset (b).

the time-independent secular potential and confirming energy conservation at the level of $10^{-3}W_0$.

Figures 3a and 3b show the maximal energy gain of the system in one collision $W_{\max}$ depending on the atom-ion mass ratio m_a/m_i and the Mathieu parameter q. The numerically calculated value for $W_{\max}$ is within a factor of two of the analytic prediction $W_{\max} = W_0 \Gamma(1/3)$. Figure 2 shows the numerically calculated total energy gain of the ion-atom system as a function of the RF phase ϕ for $q = 0.1$, $m_a = m_i/2$ (similar to the parameters in Ref. [4]). For $0 < \phi < \pi$, the system undergoes one collision after which the atom is ejected to infinity with the total energy gain ΔE well approximated by (3). For $\pi < \phi < 2\pi$, the atom remains bound to the ion until subsequent collisions add sufficient energy (on the order of W_0) to eject it. In the latter regime, ΔE depends sensitively on the RF phase at each subsequent hard-core collision spaced in time by many RF cycles, leading to a sharp dependence of ΔE on the RF phase ϕ during the initial collision.

In three-dimensional RF traps, the collision trajectory may be close to the direction where the trap confinement is only due to a DC potential, resulting in a smaller ion micromotion at the collision point. The direction of the ion's micromotion may also subtend a large angle with the collision trajectory, decreasing the work (2) done by the RF field during the collision. Together, we may expect these effects to reduce the micromotion-induced heating by a factor of order unity. To check this, numerical simulations were also done for a sample three-dimensional quadrupole RF trap from Ref. [2]. A cold ^{87}Rb atom was allowed to approach the trapped ^{174}Yb$^+$ ion from a random direction and at a random time. Figure 4b shows a sample ion-atom trajectory including multiple collisions. Due to a difference in the axial and radial frequencies of the ion trap, the collision trajectory precesses about the y axis. A histogram of the final system energies E after the atom is ejected back to infinity is shown on Figure 4a, with an average energy gain of $0.5W_0$. This confirms that the collisional heating is similar in one and three dimensions.

ion + atom		$\omega/(2\pi)$ [kHz]	q	E_s/k_B [μK]	$\hbar\omega/k_B$ [μK]	W_0/k_B [μK]
^{138}Ba$^+$	^{87}Rb [4]	200	0.11	0.052	9.6	120
^{174}Yb$^+$	^{87}Rb [2]	200	0.013	0.044	9.6	440
^{174}Yb$^+$	^{172}Yb [1]	67	0.14	0.044	3.2	34
^{174}Yb$^+$	^{40}Ca [5]	250	0.25	0.27	12	25
^{174}Yb$^+$	^{23}Na	50	0.30	0.71	2.4	1.2
^{174}Yb$^+$	^{7}Li	50	0.30	6.4	2.4	0.18

Table I: The quantum s-wave energy limit (E_s), the ion trap vibrational quantum ($\hbar\omega$), and the micromotion-induced energy scale W_0 in various ion-atom systems.

In summary, we find that, within a factor of order unity, the mean trap-induced energy gain in cold ion-atom collisions is described by the heating energy scale W_0 as given by Eq. (4). Table I shows W_0 together with the s-wave threshold energy $E_s = \hbar^2/(2\mu^2 C_4)$ and the energy $\hbar\omega$ of a trap vibrational quantum in various experimental systems. In currently realized systems, W_0 is more than one order of magnitude larger than the trap vibrational quantum and almost three orders of magnitude larger than the s-wave scattering limit. Therefore, reaching the quantum regime in close-range ion-atom collisions in these systems is unlikely.

Since, for light atoms, the ratio of of heating to the s-wave collision threshold scales as $W_0/\hbar\omega \propto (\omega C_4)^{4/3} m_a^{11/3}/m_i$ and the ratio of heating to the trap vibration quantum scales as $W_0/\hbar\omega \propto (\omega C_4)^{1/3} m_a^{5/3}/m_i$, our model predicts that micromotion heating could be mitigated using light atoms and heavy ions trapped in weak RF traps. In particular, the Yb$^+$/Li system may enter the quantum regime of direct collisions without impediment from micromotion-induced collisional heating. Heating effects described in this paper could be avoided if the atom was kept away from the ion at a distance larger than R (R=50-90 nm in current systems) such that their motion remains adiabatic relative to the RF field, e.g. by using a strong optical lattice. Another option may be the use of an optical trap for the ion, as was recently demonstrated [22].

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