Atom cooling by non-adiabatic expansion

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Motivated by the recent discovery that a reflecting wall moving with a square-root in time trajectory behaves as a universal stopper of classical particles regardless of their initial velocities, we compare linear in time and square-root in time expansions of a box to achieve efficient atom cooling. For the quantum single-atom wavefunctions studied the square-root in time expansion presents important advantages: asymptotically it leads to zero average energy whereas any linear in time (constant box-wall velocity) expansion leaves a non-zero residual energy, except in the limit of an infinitely slow expansion. For finite final times and box lengths we set a number of bounds and cooling principles which again confirm the superior performance of the square-root in time expansion, even more clearly for increasing excitation of the initial state. Breakdown of adiabaticity is generally fatal for cooling with the linear expansion but not so with the square-root expansion.

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Cooling and trapping of atoms has been a central theme in physics for over 30 years, because of applications in precision measurements and fundamental physics.\textsuperscript{[1]} Stopping particles released from an oven or source continuously or in pulses is frequently one of the steps in a cooling process.\textsuperscript{[2, 3, 4]} In this regard, a relevant and surprising recent discovery is that a reflecting potential (or “mirror” hereafter) moving with a square-root in time (square-root for short) trajectory stops all classical particles released from a point source irrespective of their initial velocity.\textsuperscript{[5]} This is in clear contrast with a linear in time (linear for short) mirror trajectory which only stops particles with one specific velocity. Motivated by this result, and by the similar behavior found for quantum wavepackets,\textsuperscript{[3]} we investigate here the effect of expanding a square box with linear or square-root wall trajectories on the average energy of a confined atom, see Fig.\textsuperscript{[1]} This is a non-trivial extension of the one-wall configuration since the confinement may induce multiple atom-wall collisions.

A given cooling objective may be achieved with an “adiabatic” expansion, see\textsuperscript{[6, 7]} as a sample of earlier and recent experiments, in which the confining walls move slowly keeping the populations of instantaneous levels constant.\textsuperscript{[1]} Adiabatic expansions constitute a traditional phase-space-conserving cooling method. Note that cooling is frequently associated with phase-space compression but in fact compression is only required for specific purposes, most notably to achieve Bose-Einstein condensates. For many applications in interferometry and metrology, and in particular in time-frequency metrology, an ultracold gas is by now preferable to condensates, to avoid the perturbing effects of interactions, or phase separation phenomena.\textsuperscript{[9]} Evaporative cooling is moreover a highly inefficient process based on losing the fastest atoms whereas a cooling expansion may retain all initial atoms. The linear expansion could lead to vanishing energy in an infinitely slow expansion, but “time” is in general a scarce commodity in the laboratory. An experiment with cold atoms is limited by the finite time in which the atoms remain trapped due, for example, to three-body losses. Moreover for applications such as pulse formation in atomic clocks, it is desirable to cool the atoms, without forming a condensate, in a short time. This increases the flux that crosses the Ramsey fields, but it also goes against adiabaticity. In this work we shall provide a way out: finite-time expansions achieving efficient cooling are possible by using fast, square-root wall trajectories that do not obey at all the adiabaticity criterion.

A number of results on expanding and contracting boxes are known in the context of chaotic dynamics and the Fermi-Ulam model\textsuperscript{[10]}, which consists of a bouncing ball between a fixed wall and a periodically moving wall $L(t)$. A related question after the pioneering work of Doescher and Rice\textsuperscript{[11]} is to find functions $L(t)$, not necessarily periodic, so that the corresponding Schrödinger equation can be solved exactly\textsuperscript{[12]}. They found explicit solutions for $L(t) = (at^2 + 2bt + c)^{1/2}$ keeping the coefficient combination $ac - b^2$ constant\textsuperscript{[12]}. The linear expansion corresponds to making this constant zero, whereas $a = 0$

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\textsuperscript{[1]} This is the standard definition of “adiabatic” in quantum mechanics, in contrast to the thermodynamical definition associated with no heat exchange. For a connection see\textsuperscript{[8]}. 
is the signature of a square-root expansion. Under these conditions, the propagator can be explicitly written in terms of known “expanding modes” $\phi_n(t)$, see e.g. 14 for details.

For our purpose here the main result of Berry and Klein 12 is that the energy of any expanding mode, $\langle \phi_n(t) | H | \phi_n(t) \rangle$ goes to zero at large time for $a = 0$ (square-root expansion), but in general it tends to a constant proportional to $a$. If we note, in addition, that non-diagonal elements of the Hamiltonian matrix in this basis tend to zero asymptotically, the conclusion is that a square-root expansion produces at long time a state with vanishing energy, whereas for a linear one there will remain a non-zero residual energy. In the expanding box these are rather intuitive results, since one expects that for any finite constant-velocity expansion, there will be low atomic velocity components that cannot interact with the moving wall, whereas the square-root mirror keeps slowing down and interacts eventually with all components. This may be seen in the final energy values of Fig. 2b for rubidium-87, which we shall comment in more detail later on.

Similarly to the time limitations mentioned before, space is also bounded in practice. It is thus desirable to examine the effect of expansions for given final box length $L_f$ and time $t_f$.

Consider the atoms in a quantum box with a moving hard wall as shown in Fig. 1. The two different trajectories for the “moving mirrors” are

$$L(t) = \begin{cases} L_0 + [(L_f - L_0)/t_f]t & \text{(linear mirror)} \\ \sqrt{L_0^2 + [(L_f^2 - L_0^2)/t_f]t} & \text{(square-root mirror)} \end{cases}$$

where $L_0$ is the initial width of the box. It is convenient to expand the wave function at an arbitrary time $t$ in the

**FIG. 1:** (Color online) (a) Scheme of atom cooling by expanding a box. (b) The two right-wall trajectories considered in this work: linear mirror (dotted blue line) and square-root mirror (solid red line), see eq. (1).

**FIG. 2:** (Color online) Dependence of the average energy $\langle E \rangle$ on the time $t$: square-root mirror (solid red line), linear mirror (dashed blue line); adiabatic energies $E_n(t)$: square-root mirror (dot-dashed red line), linear mirror (dotted blue line); (a) $t_f = 0.3$ s, $L_f = 100$ μm, (b) $t_f = 1$ s, $L_f = 50$ μm, in this figure part the adiabatic energies for the linear mirror are indistinguishable from the corresponding average energy in the scale of the figure; $L_0 = 3$ μm, initial state: ground state ($n = 1$); in all figures we use the mass of 87Rb atoms.

“instantaneous” basis $\{u_n(t)\}_{n=1,2,\ldots}$, as

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n(t) u_n(x,t) \exp \left[ (i\hbar)^{-1} \int_0^t E_n(t') dt' \right],$$

where the instantaneous eigenstate of the box Hamiltonian is $u_n(x,t) = \sqrt{\frac{2}{L(t)}} \sin \left( \frac{n\pi x}{L(t)} \right)$, and the coefficients $a_n(t)$ are determined by solving the system of differential equations that results from substituting $\psi$ into the Schrödinger equation.

The average energy can be easily calculated as

$$\langle E(t) \rangle = \sum_{n=1}^{\infty} p_n(t) E_n(t),$$

where $p_n(t) = |a_n(t)|^2$ is the population of the instantaneous eigenstate $n$, and $E_n(t) = \frac{n^2 \pi^2 \hbar^2}{2mL(t)^2}$. If the cooling objective is to diminish $\langle E \rangle$ up to a given value or to a fraction of its initial value for finite $t_f$ and $L_f$, a number of principles and bounds that govern the expansion process provide useful guidance. We shall first note some general principles and then specific bounds that underline the usefulness of the square-root versus the linear mirror:

(i) **General principles.** First, it is clear that a sudden expansion is useless. If the mirror moves too fast the
particle expands freely and the final energy \( E_f = \langle E(t_f) \rangle \) will be equal to the initial energy, \( E_i = \langle E(0) \rangle \).

Moreover, the energy bound
\[
\langle E(t) \rangle \geq E_1(t) = \frac{\pi^2 \hbar^2}{2mL^2(t)}
\]
(4)
is always fulfilled. As an application, it sets a bound on the minimal final length for a given cooling objective,
\[
L_f \geq \frac{\pi \hbar}{\sqrt{2mL_f}}.
\]
(5)

For example, if a 1/100 energy reduction is required starting from the ground state, the final length of the box should satisfy \( L_f \geq 10L_0 \).

Last but not least, the microscopic “minimal work principle” \cite{18} states that the average energy satisfies \( \langle E \rangle \geq E_{\text{adiab}} \), where the “adiabatic energy” is \( E_{\text{adiab}}(t) = \sum_n p_n(0)E_n(t) \), provided the initial state is passive (diagonal density matrix with \( p_n \geq p_{n+1} \)) and there are no level crossings. These conditions are satisfied for an expanding box and for the ground state as initial state. An exception to the principle for a nonpassive, excited initial state, will be commented later on.

\( \text{(ii) Stoppable and unstoppable velocities.} \) Classically, a necessary condition for stopping is that the particle has reached the mirror before \( t_f \). This implies a (classical) minimal stoppable velocity for the linear mirror as well as the square-root mirror (see also Fig. 1b),
\[
v_{\text{min}} = \frac{L_f}{t_f},
\]
(6)

which should be small compared to the typical velocities of the initial state. For the ground state, and using the quasi-velocity \( v_1 = \pi \hbar / (mL_0) \) for an estimate, this gives the condition
\[
\frac{v_{\text{min}}}{v_1} = \frac{mL_fL_0}{t_f \pi \hbar} \ll 1 \iff \frac{mL_fL_0}{\pi \hbar} \ll t_f,
\]
(7)

with different implications for the two cases: the square-root mirror stops (for \( L_0/L_f \rightarrow 0 \)) all classical particles moving with velocity greater than \( v_{\text{min}} \), whereas this is not true for the linear mirror.

\( \text{(iii) Condition of adiabaticity.} \) To maintain adiabaticity during the expansion, the system should satisfy
\[
\frac{|\langle u_k(t) | \frac{\partial}{\partial t} u_n(t) \rangle|}{\langle E_k(t) - E_n(t) \rangle / \hbar} \ll 1
\]
(8)

for populated levels and their neighboring levels \cite{17}. Applying this to the expanding box for \( k = 2 \) and \( n = 1 \) at \( t_f \), when the levels are at closest distance from each other,
and neglecting $L_0/L_f$ terms, we get

\[
\frac{8}{9\pi} \frac{mL_f^2}{\hbar} < t_f
\]

(9)
or $t_f E_{\text{adiab}}(t_f) > \frac{4}{\pi} \hbar$, which is - because of $L_0 \ll L_f$ - a stronger condition than the condition (7) for the square-root mirror. Earlier breakdown of adiabaticity for the linear mirror results, in accordance with the Berry-Klein asymptotics, in a finite final energy, whereas, as we shall see, the square-root mirror provides efficient cooling as long as the stopping condition is satisfied, irrespective of adiabaticity.

For sufficiently large $t_f$ and small $L_f$, the whole expansion can be adiabatic, even for the square-root case, as in Fig. 2b. In adiabatic processes like the one depicted, the square-root mirror makes a faster approach to the final energy than the linear one, as a consequence of the inequality $L_{\text{square-root}}(t) \geq L_{\text{linear}}(t)$.

To determine how much shorter the expansion time $t_f$ could be, we compare in Fig. 3a for the atom initially in the ground state, the final average energies with respect to $t_f$ with a fixed $L_f$. The square-root is always more efficient than the linear mirror. In particular at $t_f = 0.3$ s a 1/100 reduction of the initial energy is achieved. Fig. 2b provides details of the evolution for that particular final time. The expansion for the linear mirror is adiabatic only up to some time $(\approx 0.015$ s), and in the final stage of the evolution the constant energy value predicted asymptotically by Berry and Klein is reached. On the other hand, the square-root mirror expansion is never adiabatic. Efficient cooling starts at time $\tau_C \approx 0.02$ s, and this delay may be understood classically since the square-root mirror is quite fast at first so that the particles need some time to catch up with the mirror. In spite of the lack of adiabaticity, the stopping criterion (7) is well satisfied, so that the end result is a very fast and efficient cooling. Note that the minimal work principle is respected at all times.

Finally, we compare the behavior of different initial states. Fig. 4a shows the average energy for different initial states, $n = 1, 2, 3$. When the initial state is an excited state, the density matrix is not passive: this allows $\langle E \rangle < E_{\text{adiab}}$ to occur, a (justified) transient violation of the microscopic minimal work principle, see the inset of Fig. 4b. Moreover one notes in Fig. 4c that the difference between the curves for square-root and linear expansions for short $t$ increases with the excitation.

This suggests a good behavior of the square-root expansion also for simple systems such as a polarized Fermi gas, or its (symmetrized) bosonic counterpart, the Tonks-Girardeau gas. The average energy of a Tonks-Girardeau gas [14] with $N$ particle is given by $\langle E \rangle = \sum_{n=1}^{N} \langle E \rangle_n$ where $\langle E \rangle_n$ is the average energy of the single-particle solution with initial state $u_n$. In Fig. 3b, we compare the average energy of the square-root and the linear mirror for a Tonks-Girardeau gas with 5 particles for different final times $t_f$.

In conclusion, square-root in time box expansions offer advantages over linear in time expansions, allowing faster and more efficient cooling. While the breakdown of adiabaticity is generally fatal for cooling with the linear expansion, this is not the case for square-root expansion. The universal stopping and cooling properties of square-root expansions are also in contrast to generic state-dependence of variational methods. We close noticing that the box studied can be realized experimentally in an all-optical implementation [20]. The effect of alternative trapping potentials and mirror trajectories as well as further many-body effects will be reported elsewhere.

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