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REVIEW ARTICLE

Shortcut to adiabaticity in harmonic traps

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Abstract. We review the methods to preserve the initial state populations in a fast harmonic trap expansion. The design of the time dependence of the frequency using inverse techniques presents advantages over the slow adiabatic approach, band-bang methods, or the non-local "transitionless tracking" algorithm. Many operations with cold atoms make use of adiabatic expansions and may benefit from such a shortcut to adiabaticity.

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1 Introduction

A standard operation to probe, control, or prepare a quantum system, in particular in the realm of atomic and molecular science, consists in changing the external parameters of the Hamiltonian. In many cases the ideal transformations from an initial to a final parameter configuration are the ones that do not induce any transitions [1,2]. The standard solution to this requirement is to perform the changes "adiabatically". Most experiments with cold atoms are based on a cooling stage and then an adiabatic drive of the system to some desired final trap or regime [3]. The adiabatic step may have different objectives, such as the reduction of velocity dispersion and collisional shifts for spectroscopy and atomic clocks [4], reaching extremely low temperatures unaccessible by standard cooling

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techniques [5], or, in experiments with optical lattices, broadening the state before turning on the lattice [6]. There is recently a surge of interest in adiabatic theory and applications for fundamental reasons [1,3], and also in connection with quantum information [7,8]. In adiabatic processes the system follows slowly at all times the instantaneous eigenvalues and eigenstates of the time-dependent Hamiltonian. The main problem is that the long times needed can make them useless or impractical [3], or quite simply a faster process is preferred, e.g., to increase the repetition rate of a cycle.

A highly desirable goal is to achieve the same final state as the slow adiabatic processes, possibly up to phase factors, but in a much shorter time, in other words, to find a shortcut to adiabaticity. Moreover the procedure should work for arbitrary initial states, and be realizable in practice. This goal is also relevant to optimize the passage between two thermal states of a system [9–12], a long standing question in the fields of optimal control theory and finite time thermodynamics. For time-dependent harmonic oscillators, minimal times have been established using "bang-bang" real-frequency processes believed up to now to be optimal [11], in which the frequencies are changed suddenly at certain instants but kept constant otherwise.

In this paper, we shall review different shortcuts to adiabaticity that have been proposed recently to change a harmonic Hamiltonian frequency in a finite time t_f. One approach is to design appropriate "parameter trajectories" of the frequency from the initial to the final values using bang-bang techniques [11]. Another method is to design appropriate "parameter trajectories" of the frequency based on Lewis-Riesenfeld invariants of motion [15] supplemented by simple "inverse-problem" techniques [16]. We shall call this approach "inverse-invariant" method, or II for short [13, 14]. A third approach for getting shortcuts to adiabaticity is to apply a new interaction that modifies the Hamiltonian beyond a simple parameter evolution of the original harmonic form. This option, termed "transitionless-tracking" approach, or TT for short, relies on a general framework set by Kato in a proof of the adiabatic theorem [17], and has been formulated recently by Berry [1].

We shall review first the "inverse-invariant" method in Section 2, comparing it with adiabatic and bang-bang techniques. This method will be applied to Bose-Einstein condensates governed by the Gross-Pitaevskii (GP) equation in Section 3. The TT method is reviewed in Section 4.

2 Fast optimal frictionless atom cooling in harmonic traps

2.1 "Inverse-Invariant" method

For simplicity, we shall firstly describe our method for states representing single atoms of mass m. Consider an effectively one-dimensional time-dependent harmonic oscillator,

$$H=\frac{1}{2m}\hat{p}^2+\frac{1}{2}m\omega^2(t)\hat{q}^2, \tag{1}$$

with an initial angular frequency $\omega(0)>0$ at time $t=0$ and final frequency $\omega_f=\omega(t_f)<\omega(0)$ at time t_f. When the Hamiltonian is constant we are used to think of temperature changes and "cooling" in terms of population changes. Note however that when the Hamiltonian changes with time the temperature may change even if the populations stay constant. For a population preserving process involving canonical states

$$e^{-H/(kT)}/\mathrm{tr}\left[e^{-H/(kT)}\right],$$

the decrease in frequency may be considered as a "cooling" process since the initial and final partition functions are the same, thus

$$\frac{E_n(0)}{kT(0)}=\frac{E_n(t_f)}{kT(t_f)}, \tag{2}$$

which implies a temperature reduction $T(t_f)=T(0)\omega_f/\omega(0)$. This process though, does not involve a phase-space compression. (A process in which, in addition to a temperature decrease there is phase-space compression is sometimes called "brightening" or "true cooling" [18].)

The challenge is to find a trajectory $\omega(t)$ between these two values so that the populations of the oscillator levels $n=0,1,2...$ at t_f are equal to the ones at $t=0$. Our tool to engineer $\omega(t)$ and the state dynamics will be the solution of the corresponding Schrödinger equation based on the invariants of motion [15, 19–21] of the following form

$$I(t)=\frac{1}{2}\left[(1/b^2)\hat{q}^2 m\omega_0^2+\frac{1}{m}\hat{\pi}^2\right], \tag{3}$$

where $\hat{\pi}=b\hat{p}-m\dot{b}\hat{q}$ plays the role of a momentum conjugate to $\hat{q}/b$, the dots are derivatives with respect to time, and ω_0 is in principle an arbitrary constant. The invariance condition reads

$$\frac{dI}{dt}\equiv\frac{\partial I}{\partial t}+\frac{1}{i\hbar}[I,H]=0, \tag{4}$$

and implies for the scaling, dimensionless function $b=b(t)$ the subsidiary condition

$$\ddot{b}+\omega^2(t)b=\frac{\omega_0^2}{b^3}, \tag{5}$$

which is an Ermakov equation where real solutions must be chosen to make I Hermitian [22]. The form of the invariant (3) and the subsidiary condition (5) follow by inserting an ansatz quadratic in $\hat{p}$ and $\hat{q}$ into (4).

Whereas ω_0 is frequently rescaled to unity by a scale transformation of b [15], other convenient choice is $\omega_0=\omega(0)$ as we shall see below. $I(t)$ has the structure of a harmonic oscillator Hamiltonian as well (as long as $\omega_0^2>0$), with time-dependent eigenvectors $|n(t)\rangle$ and time-independent eigenvalues $(n+1/2)\hbar\omega_0$. They are useful because

the general solution of the Schrödinger equation can be written as a superposition of orthonormal "expanding modes"

$$\psi(t,x)=\sum_n c_n e^{i\alpha_n(t)}\langle x|n(t)\rangle, \tag{6}$$

where

$$\alpha_n(t)=-(n+\frac{1}{2})\omega_0\int_0^t\frac{dt'}{b(t')^2},$$

and the c_n are time independent amplitudes that may be computed at $t=0$. For a single mode and $\omega_0^2>0$,

$$\Psi_n(t,x)=\left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4}\frac{\exp(\alpha_n(t))}{\sqrt{(2^n n!b(t))}}\exp\left[\frac{im}{2\hbar}\left(\frac{\dot{b}}{b(t)}+\frac{i\omega_0}{b(t)^2}\right)x^2\right]\widetilde{H}_n\left[\sqrt{\left(\frac{m\omega_0}{\hbar}\right)}\frac{x}{b(t)}\right], \tag{7}$$

where $\widetilde{H}_n$ are the Hermite polynomials. The corresponding time-dependent average energy is given by

$$\langle H(t)\rangle_n=\frac{(2n+1)\hbar}{4\omega_0}\left(\dot{b}^2+\omega^2(t)b^2+\frac{\omega_0^2}{b^2}\right). \tag{8}$$

The average position of an expanding mode is zero and the standard deviation $\sigma=(\int dx x^2|\Psi_n|^2)^{1/2}$ is proportional to b, $\sigma=b(n+1/2)^{1/2}/(m\omega_0/\hbar)^{1/2}$, so that the scaling factor provides a measure of the state width along its evolution.

The case in which the frequency is scaled as

$$\omega(t)=\omega(0)/b^2, \tag{9}$$

with $b=(At^2+2Bt+C)^{1/2}$ has been much studied [19, 20, 23]. Substituting this into Eq. (5) gives $\omega_0^2=\omega(0)^2+AC-B^2$. For a hard wall trap, the square-root-in-time scaling factor b, corresponding to $A=0$, has been shown to provide fast and efficient cooling [24, 25]. However, for harmonic traps, much more commonly realized in ultracold experiments, such time dependence leads to negative values of ω_0^2 even for modest cooling objectives. Note that, using (9) at $t=0$ and t_f with $A=0$, it follows that

$$C=1 \quad \text{and} \quad B=\frac{\omega(0)-\omega_f}{2t_f\omega_f}.$$

Thus ω_0^2 becomes negative easily by decreasing t_f. This is cumbersome because the reference or auxiliary system provided by the invariant is not a harmonic oscillator with discretized levels but a harmonic repeller, so Eq. (7) becomes invalid. Moreover, instead of (6), linear combinations of a continuum of non-square-integrable expanding modes would be needed to describe the evolution of any single eigenstate of the initial trap. This is of course only a drawback to calculate the dynamics using the invariant, not to realize the expansion in the laboratory. In fact for a negative ω_0^2 it is more convenient to

use the adiabatic basis [26]. The numerical results show that, even though the square-root-in-time scaling is singularly efficient for adiabatic following, as discussed below, the cooling performance fails for very short expansion times t_f.

An alternative, successful strategy is to set $\omega_0 = \omega(0)$ (this will be the case from now on) and apply inverse scattering techniques for complex potential optimization [16, 27, 28], leaving $\omega(t)$ undetermined at first and imposing boundary conditions (BC) on b and its derivatives at $t=0$ and t_f, to assure: (a) that any eigenstate of $H(0)$ evolves as a single expanding mode and that (b) this expanding mode becomes, up to a position-independent phase factor, equal to the corresponding eigenstate of the Hamiltonian $H(t_f)$ of the final trap. In this way the populations in the instantaneous basis will be equal at initial and final times. $b(t)$ may be chosen as a real function satisfying the BC, for example a polynomial or some other convenient functional form with enough free parameters. After $b(t)$ has been engineered, the physical frequency $\omega(t)$ is given by Eq. (5). The resulting Hamiltonian in (1) will be called H_{II} if we need to distinguish it from other options.

BC at $t=0$: We choose $b(0)=1$, $\dot{b}(0)=0$ so that $H(0)$ and $I(0)$ commute and have common eigenfunctions. Since $\omega_0=\omega(0)$, $\ddot{b}(0)=0$ must hold as well. These BC imply that any initial eigenstate of $H(0)$, $u_n(0)$, will evolve according to the expanding mode (7) for all later times. In general $H(t)$ and $I(t)$ do not commute for $t>0$, so that the expanding mode $\Psi_n(t)$ may have more than one component in the "adiabatic basis" of instantaneous eigenstates of $H(t)$, $\{u_n(t)\}$, $n=0,1,2...$, where

$$u_n(t,x)=\left(\frac{m\omega(t)}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\exp\left(-\frac{m}{2\hbar}\omega(t)x^2\right)\tilde{H}_n\left(\sqrt{\frac{m\omega(t)}{\hbar}}x\right). \tag{10}$$

BC at $t=t_f$: We want $\Psi_n(t_f)$ to be proportional, up to the global phase factor $e^{i\alpha_n(t_f)}$, to the eigenstate of the final trap $u_n(t_f)$. Thus we impose

$$b(t_f)=\gamma=(\omega_0/\omega_f)^{1/2},\quad \dot{b}(t_f)=0,\ \ddot{b}(t_f)=0.$$

We may see as well that these boundary conditions minimize the average energy. From Eq. (8), one finds $\langle H(t_f)\rangle_n$ in terms of $b_f=b(t_f)$ and $\dot{b}_f=db(t)/dt|_{t=t_f}$,

$$\langle H(t_f)\rangle_n=\frac{(2n+1)\hbar}{4\omega_0}\left(\dot{b}_f^2+\omega_f^2 b_f^2+\frac{\omega_0^2}{b_f^2}\right). \tag{11}$$

Since b_f and $\dot{b_f}$ can be set independently we can minimize the terms depending on them separately,

$$\frac{\partial\langle H(t_f)\rangle_n}{\partial\dot{b}_f}=\frac{(2n+1)\hbar}{2\omega_0}\dot{b}_f=0, \tag{12}$$

$$\frac{\partial\langle H(t_f)\rangle_n}{\partial b_f}=\frac{(2n+1)\hbar}{4\omega_0}\left(2\omega_f^2 b_f-2\frac{\omega_0^2}{b_f^3}\right)=0. \tag{13}$$

To satisfy these equations, we have

$$\dot{b}_f = 0, \tag{14}$$

$$\omega_f^2 = \omega_0^2 / b_f^4. \tag{15}$$

Comparing (15) with the Ermakov equation at t_f, it follows that $\ddot{b}_f = 0$. In other words, the boundary conditions that we have imposed above correspond to the minimal possible average energy, which, using $\ddot{b}_f = 0$, (15) and (14) in (11) turns out to be the adiabatic energy,

$$\langle H(t_f)\rangle_n(minimal) = (n+1/2)\hbar\omega_f^2. \tag{16}$$

Since this is true for all n this means that we cannot design any trajectory to achieve an average energy below the one provided by an adiabatic process. Any other choice of boundary conditions for b would necessarily produce excitations.

It is interesting to compute the average energy as well for a density operator ϱ which is stationary in the initial trap. This means that it is diagonal in the basis of the invariant,

$$\begin{aligned}\langle H\rangle &= \mathrm{tr}[\varrho(t)H(t)] = \mathrm{tr}[\sum_n p_n|\Psi_n\rangle\langle\Psi_n|H(t)] = \sum_n p_n\langle\Psi_n|H(t)|\Psi_n\rangle \\ &= \sum_n p_n \frac{(2n+1)\hbar}{4\omega_0}\left(\dot{b}+\omega^2 b^2+\frac{\omega_0^2}{b^2}\right) \\ &= p_0 E_0(t) + \langle n\rangle_0 \frac{\hbar}{2\omega_0}\left(\dot{b}+\omega^2 b^2+\frac{\omega_0^2}{b^2}\right) \\ &= [2\langle n\rangle_{inv}+1]E_0(t),\end{aligned} \tag{17}$$

where $\langle n\rangle_{inv}$ is the average vibrational quantum number in the invariant basis. This does not change with time so it coincides with the initial average. Comparing this to the corresponding calculation in the adiabatic basis,

$$\begin{aligned}\langle H\rangle &= \sum_n p_n^{ad}\langle H\rangle_n^{ad} = \sum_n p_n^{ad}\hbar(n+1/2)\omega(t)(\langle n\rangle^{ad}+1/2)\hbar\omega(t) \\ &= (2\langle n\rangle^{ad}+1)E_0^{ad}(t),\end{aligned} \tag{18}$$

we may calculate the average excitation number in the adiabatic basis as a function of time,

$$2\langle n\rangle^{ad}+1 = \frac{\langle H\rangle}{E_0^{ad}(t)} = \frac{2\langle H\rangle}{\hbar\omega(t)} = \frac{2[2\langle n\rangle_{inv}+1]E_0(t)}{\hbar\omega(t)}. \tag{19}$$

Substituting the simple polynomial ansatz $b(t) = \sum_{j=0}^{5} a_j t^j$ into the six BC set above gives six equations that can be solved to provide the coefficients,

$$b(t) = 6(\gamma-1)s^5 - 15(\gamma-1)s^4 + 10(\gamma-1)s^3 + 1, \tag{20}$$

where $s = t/t_f$. The universality of the solution indicates that there is no fundamental limitation on t_f as long as the potential is really quadratic. At initial and final times 0 and

t_f, $\omega(t)=\omega_0/b^2(t)$, but, unlike the treatment with square-root-in-time expansions, this relation does not hold in general for an arbitrary intermediate time.

The six conditions mentioned above leave time-dependent phases $e^{i\alpha_n(t)}$ but they are irrelevant regarding the population of the nth level. In particular density operators which are stationary with respect to $H(0)$ (e.g. a pure state $|u_n(0)\rangle\langle u_n(0)|$ or a canonical state) are mapped onto the corresponding stationary states of $H(t_f)$ with the phases canceled. In other cases the phases remain but the populations are preserved. Note that $e^{i\alpha_n(t)}$, see Eq. (7), is the phase factor that the initial state $u_n(0)$ would get in a virtual adiabatic process with adiabatic (instantaneous) energy $(n+1/2)\hbar\omega_0/b^2$. The trajectories may be designed to control the phase by adding integral conditions, such as

$$\tau(t_f)=\int_0^{t_f}\frac{dt}{b^2(t)}=\frac{\omega_f}{\omega_0}t', \tag{21}$$

where t' is some desired time. This would require a more complicated ansatz for b, such as a polynomial of higher degree.

The shortcut to adiabaticity using invariants applies to arbitrary initial states, superpositions or mixed. This also means that fast frictionless cooling is directly applicable to N-body non-interacting fermions or to a Tonks-Girardeau gas [29,30].

An important feature of $\omega^2(t)$ is that it may be negative during some time interval in which the potential becomes an expulsive parabola [31]. In general the (imaginary) frequency of the repulsive region increases for shorter cooling times. For the regular Ermakov equation (5), a simple estimate for the polynomial ansatz b(t), and $\omega_0\gg\omega_f$, is that the imaginary frequencies occur if $t_f<1/(3\omega_f)$. (For a given $s=t/t_f$, a zero of $\omega^2(t)$ is found when $t_f=u(s)/\omega_f$, where $u(s)$ may be computed numerically. Its maximum value, $\sim 1/3$, occurs near $s=0.43$.) Notice that this is different from the negativity of ω_0^2 commented above. Now ω_0^2 remains positive by construction.

2.2 Comparisons with adiabatic and Bang-Bang trajectories

Whereas in principle the II method is not intrinsically limited and allows for an arbitrarily small t_f (in the purely harmonic potential, for limitations due to anharmonicity see below) we shall discuss here the limitations of adiabatic or bang-bang methods.

To maintain adiabaticity during the expansion, the system should satisfy [25]

$$\left|\frac{\langle k(t)|\partial_t n(t)\rangle}{[E_k(t)-E_n(t)]/\hbar}\right|\ll 1, \tag{22}$$

where

$$\langle k(t)|\partial_t n(t)\rangle=\begin{cases}\frac{\dot\omega}{4\omega}\sqrt{n(n-1)} & (k=n-2),\\ -\frac{\dot\omega}{4\omega}\sqrt{(n+1)(n+2)} & (k=n+2),\\ 0 & (\text{otherwise}).\end{cases}$$

For a linear ramp,

$$\omega(t) \to \omega_0 + (\omega_f - \omega_0)t/t_f,$$

the adiabaticity condition (22) for the harmonic oscillator becomes

$$|\sqrt{2}\dot{\omega}/(8\omega^2)| \ll 1. \tag{23}$$

This implies a very long time, $t_f^{(ad)} \gg 1.1$ s for an initial frequency $\omega_0 = 250 \times 2\pi$Hz, and final one $\omega_f = 2.5 \times 2\pi$Hz. In practice 6 s are necessary to achieve a 1% relative error in the final energy of the ground state with the linear ramp.

A much more efficient (still adiabatic) strategy is to distribute $\dot{\omega}/\omega^2$ uniformly along the trajectory, i.e., $\dot{\omega}/\omega^2 = c$, c being constant. By solving this differential equation and imposing $\omega_f = \omega(t_f)$ we get

$$\omega(t) = \frac{\omega_0}{1 - (\omega_f - \omega_0)t/(t_f \omega_f)}.$$

This corresponds to the case $A = 0$, $2B = -(\omega_f - \omega_0)/(t_f \omega_f)$, $C = 1$ (i.e., a square-root-in-time scaling factor), and implies $t_f^{(ad)} \gg 11$ms for the given initial and final frequencies. With this optimized adiabatic trajectory a 1% error level for the ground state energy is achieved after 45ms.

Bang-bang trajectories with real frequencies also suffer from fundamental limitations. For the three-jump trajectory [11]

$$\omega(t) = \begin{cases} \omega_0 & (t = 0), \\ \omega_1 & (0 < t < \tau_1), \\ \omega_2 & (\tau_1 < t < \tau_1 + \tau_2), \\ \omega_f & (t = t_f = \tau_1 + \tau_2), \end{cases} \tag{24}$$

the cooling is faster for smaller values of ω_1 and larger values of ω_2. In principle the fastest process to reach the target state corresponds to $\omega_1 \to 0$ and $\omega_2 \to \infty$ [11] with

$$t_f^{min} = \sqrt{\frac{1 - \omega_f}{\omega_0}} \times (\omega_f \omega_0)^{-\frac{1}{2}}, \tag{25}$$

e.g., $t_f^{min} \approx 6.3$ ms for an initial frequency $\omega_0 = 250 \times 2\pi$Hz and final one $\omega_f = 2.5 \times 2\pi$Hz.

These are results based on optimal control theory, initial and final thermal states, and the constraint $\omega_{1,2} > 0$. If the positivity condition for the intermediate frequencies is relaxed, faster processes involving finite frequencies and $t_f < t_f^{min}$ are possible, although the discontinuous jumps in this type of trajectory call into question its realizability. In any case times smaller than t_f^{min} are possible so we should revise a finite time version of the third principle (if $\omega_f \to 0$, $t_f^{min} \to \infty$ as $\omega_f^{-1/2}$) and maximal cooling rates based on t_f^{min}.

2.3 Experimental realization

Purely optical traps are manipulated in time for the adiabatic cooling of single neutral atoms [32]. We propose an experimental realization based on a time-dependent far-off resonance optical dipole trap (red detuned) and an antitrap (blue detuned), which are not sensitive to the detailed internal states and in particular to Zeeman sublevels, if sufficiently detuned from the atomic line resonance. This effective interaction can be made time dependent by varying the laser intensity, the frequency, or both [4], since the optical frequencies are many orders of magnitude larger than Rabi frequencies or detunings, and the changes will be slowly varying in the scale of optical periods. The intensity of a dipole trap can be changed by three or four orders of magnitude in 100 ns using acousto-optics or electro-optics modulators.

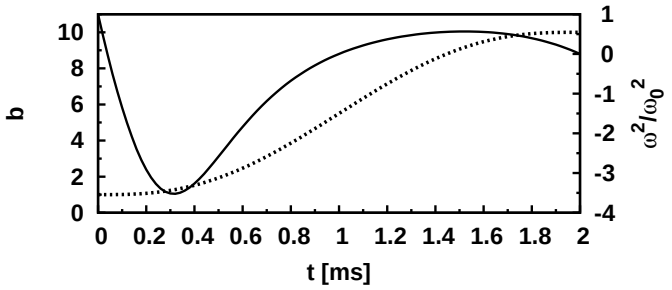
We have so far considered one dimension (1D). Formally the three coordinates in an ideal harmonic trap are uncoupled so the expansion processes can be treated independently, but, in practice changing the intensity of a laser beam affects simultaneously the longitudinal and transversal frequencies. To avoid this problem, the degrees of freedom available, laser intensities and waists [33], may be used to satisfy the desired frequency trajectory in one coordinate, say longitudinal, while keeping the other frequency constant. It is also possible to leave the waists constant and add more lasers to compensate for the transversal frequency change. In the above optical implementation of the potential we also have to take into account the anharmonicity and finite depth as they limit the possible excitation of the (initial and final) states. In Fig. 1, an example for a fast optimal frictionless atom cooling is shown. Fig. 1(a) displays $b(t)$ and the resulting $\omega^2(t)$ leading to an optimal cooling in exact harmonic traps and Fig. 1(b) presents snapshots of the corresponding time evolution of the wave function (dotted lines). In addition, the time evolution is presented if the harmonic potential is approximated by a Gaussian (solid lines). The final wave functions are nearly indistinguishable in the two cases. The fidelity, i.e., the overlap between the final state using an exact harmonic potential and using a Gaussian, is $F=0.91$ in this case.

One may study as well magnetic implementations. In magnetic traps, the frequency has been modulated harmonically to look for collective excitation modes of a condensate [34], and ramped down adiabatically to change its conditions (critical temperature, particle number, spatial extension) [34,35]. Some experiments involve both time-dependent magnetic and optical traps or antitraps [36].

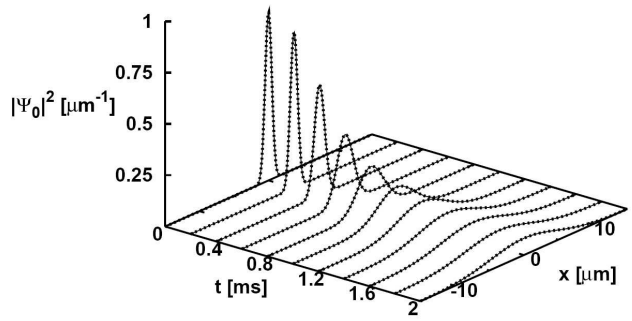
3 Application to Bose-Einstein condensates

In this section, we adapt the former results to Bose-Einstein condensates governed by the Gross-Pitaevskii equation in different dimensions using self-similarity [37].

As we shall see, the applicability of the method will depend critically on the effective dimension of the trap. By 1D traps we mean here quasi-1D cigar-shaped traps with tight (fixed) transversal confinement where the axial frequency is varied in time; 2D traps are



(a)



(b)

Figure 1: Example of fast optimal frictionless atom cooling: $\omega_0 = 250\times 2\pi$Hz, $\omega_f = 2.5\times 2\pi$Hz, mass of Rb-87, and $t_f = 2$ms. (a) $b(t)$ (dotted line, left axis) and $\omega^2(t)$ (solid line, right axis). (b) Time evolution of $|\Psi_0(t,x)|^2$ with a harmonic potential $V(t,x) = m\omega^2(t)x^2/2$ (dotted line) and with a Gaussian potential $V(t,x) = mw^2\omega^2(t)\left(1-\exp\left(-(2x^2/w^2)\right)\right)/4$ of width $w = 50\mu$m (solid line, indistinguishable from the dotted line); in both cases: the function $\omega^2(t)$ shown in (a) is used, the initial state at $t=0$ is the ground state of the harmonic potential.

quasi-2D disk-shaped traps with tight, fixed, axial confinement in which the transversal frequency is varied; and the 3D traps refer to harmonic traps with spherical symmetry. We assume in all cases that a GP equation can be derived corresponding to each dimensionality, and use g generically for the coupling parameter of the non-linear term even though it is different for the three cases [38]. We shall discuss 1D traps first for simplicity, and then 2D and 3D traps.

3.1 One dimensional traps

The effective 1D Gross-Pitaevski equation for the longitudinal (x) direction in an elongated cigar trap is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega(t)^2x^2 + g|\psi|^2\right]\psi, \tag{26}$$

g being the coupling parameter. The application of the invariant concept here is not as simple as for the Schrödinger equation [39]. Instead, we shall use an approach which leads in that case to the same results. The basic idea is to assume for the ansatz [40]

$$\psi(x,t)=e^{-\beta(t)}e^{-\alpha(t)x^2}\phi(x,t). \tag{27}$$

Substituting this into Eq. (26), and using the scaling $\rho=x/b$ and redefined wavefunction $\Phi(\rho,t)=\phi(x,t)$, we get

$$\begin{aligned} i\hbar\frac{\partial\Phi}{\partial t}=&-\frac{\hbar^2}{2m}\frac{1}{b^2}\frac{\partial^2\Phi}{\partial\rho^2}+\left[\frac{1}{2}m\omega(t)^2+i\hbar\dot{\alpha}-\frac{2\hbar^2}{m}\alpha^2\right]b^2\rho^2\Phi \\ &+\left[ge^{-(\alpha+\alpha^*)x^2}e^{-(\beta+\beta^*)}|\Phi|^2\right]\Phi+\left[i\hbar\dot{\beta}+\frac{\hbar^2\alpha}{m}\right]\Phi+\left[2\frac{\hbar\alpha}{m}+i\frac{\dot{b}}{b}\right]\hbar\rho\frac{\partial\Phi}{\partial\rho}, \end{aligned} \tag{28}$$

where the dot means as before derivative with respect to time. If we impose that the coefficients in square brackets [...] of the last two terms vanish (we assume b real),

$$\beta=\frac{1}{2}\ln b,\qquad \alpha=-\frac{im}{2\hbar}\frac{\dot{b}}{b}, \tag{29}$$

and

$$e^{-(\alpha+\alpha^*)x^2}e^{-(\beta+\beta^*)}=b^{-1}.$$

Suppose now that the coefficient of $b^2\rho^2\Phi$ in (28) is made constant, equal to $m\omega_0^2/(2b^4)$ (for an alternative see the final discussion). As in the previous section $\omega_0=\omega(0)$. Using (29) this is equivalent to imposing for b and $\omega(t)$ the same Ermakov equation as Eq. (5), $\ddot{b}+\omega(t)^2b=\omega_0^2/b^3$. We may express the resulting wave equation in terms of a new scaled time,

$$\tau(t)=\int_0^t\frac{dt'}{b(t')^2}, \tag{30}$$

and wavefunction $\Psi(\rho,\tau)=\phi(\rho,t)$,

$$i\hbar\frac{\partial\Psi}{\partial\tau}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial\rho^2}+\frac{m\omega_0^2}{2}\rho^2\Psi+gb|\Psi|^2\Psi. \tag{31}$$

This is the Schrödinger equation of a time-independent harmonic oscillator if $g=0$ and corresponds to the case discussed in the previous section, which may be handled with the boundary conditions

$$b(0)=1,\quad \dot{b}(0)=0, \tag{32}$$

$$b(t_f)=(\omega_0/\omega_f)^{1/2},\quad \dot{b}(t_f)=0, \tag{33}$$

for the scaling factor.

If $g \neq 0$ the coefficient of the non-linear term in the auxiliary equation is generally time dependent. The consequence is that imposing $\dot{b}(t_f) = 0$ eliminates the phase-factor $e^{-\alpha(t_f)x^2}$ but nothing guarantees that $\Psi(\tau(t_f))$ is proportional to the instantaneous eigenstate of the GP equation at t_f. One could in principle make the coupling coefficient time-dependent with the aid of a Feshbach resonance as $g(t) = g_0/b(t)$, with g_0 constant. The auxiliary equation has then time-independent coefficients,

$$i\hbar\frac{\partial\Psi}{\partial\tau} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial\rho^2} + \frac{m\omega_0^2}{2}\rho^2\Psi + g_0|\Psi|^2\Psi. \tag{34}$$

It can be solved as $e^{-i\mu\tau(t)/\hbar}\Psi(x/b,0)$, μ being the chemical potential for the initial trap, so that

$$\psi(x,t) = b^{-1/2}e^{\frac{im}{2\hbar}\frac{\dot{b}}{b}x^2}e^{-i\mu\tau(t)/\hbar}\Psi(x/b,0), \tag{35}$$

and the inverse method described for the Schrödinger equation can now be applied to design a fast process for the ground state condensate. Keeping $b(t) = b_f$ constant for $t > t_f$, which results in

$$\omega(t) = \omega_f \text{ and } g = g_0(\omega_f/\omega_0)^{1/2} \text{ for } t > t_f,$$

the solution $\psi(x,t)$ of (26) given by (35) becomes stationary, and the new scaled chemical potential is $\mu/b(t_f)^2$.

Other special case is a "Thomas Fermi" (TF) limit, keeping g constant. Using a modified Ermakov equation and a different time scaling

$$\ddot{b} + \omega(t)^2 b = \frac{\omega_0^2}{b^2}, \qquad \tau(t) = \int_0^t \frac{dt'}{b(t')}, \tag{36}$$

render an auxiliary equation with time-independent coefficients for the non-linear and harmonic potential terms. If $g|\Psi|^2/(\hbar\omega_0) \gg 1$, the kinetic term may be neglected,

$$i\hbar\frac{\partial\Psi}{\partial\tau} = \frac{m\omega_0^2}{2}\rho^2\Psi + g|\Psi|^2\Psi. \tag{37}$$

This equation can be solved by separation of variables, $\Psi(x/b,\tau) = e^{-i\mu\tau/\hbar}\Psi(x/b,0)$, and $\psi(x,t)$ takes again the form of Eq. (35), with different values for μ, τ, b, and the initial wavefunction. This TF approximation is carried out in the auxiliary equation, and not at the level of the original GP equation, since that would imply a frozen density [37, 40]. Applying the modified Ermakov equation in (36), the inversion method to find $\omega(t)$ requires in this 1D-TF scenario to change the boundary condition at t_f in (33) to $b(t_f) = (\omega_0/\omega_f)^{2/3}$, with $\ddot{b}(0) = \ddot{b}(t_f) = 0$ as before.

3.2 Two and three dimensional traps

A wavefunction ansatz [37] that guarantees an auxiliary equation without first spatial derivatives is

$$\psi(\mathbf{r},t)=b^{-d/2}\exp(\frac{imr^2}{2\hbar}\frac{\dot{b}}{b})\phi(\mathbf{r},t), \tag{38}$$

where d is the dimension, $r=(x^2+y^2)^{1/2}$ in 2D or $r=(x^2+y^2+z^2)^{1/2}$ in 3D.

Substituting (38) into the 2D or 3D GP equations, with $\boldsymbol{\rho}=\mathbf{r}/b$ and a notation for the wavefunctions parallel to the 1D case there results

$$i\hbar\frac{\partial\Psi}{\partial\tau}\left(\frac{d\tau}{dt}b^2\right)=-\frac{\hbar^2}{2m}\Delta_\rho\Psi+\frac{m}{2}\left[\omega^2(t)+\frac{\ddot{b}}{b}\right]\rho^2b^4\Psi+\frac{g}{b^{d-2}}|\Psi|^2\Psi, \tag{39}$$

where $\Psi=\Psi(\boldsymbol{\rho},\tau)$, τ has not been specified yet and the Laplacian should be adapted to the dimension. This equation includes the case $d=1$ by substituting the Laplacian by a second derivative and $r\to x$.

In 2D, the ordinary Ermakov equation (5) and the τ in Eq. (30) are the optimal choice because all coefficients in the auxiliary equation (assuming a constant g) become time independent. This is so even outside the Thomas-Fermi regime,

$$i\hbar\frac{\partial\Psi}{\partial\tau}=-\frac{\hbar^2}{2m}\Delta_\rho\Psi+\frac{m\omega_0^2}{2}\rho^2\Psi+g|\Psi|^2\Psi. \tag{40}$$

Now a frictionless process can be designed by shaping b and ω exactly as in the 1D Schrödinger equation, i.e., using (32) and (33).

The case $d=3$ is similar to 1D since the generic case leads to time-dependent coefficients in the auxiliary equation. As in the 1D case, by using Eqs. (5) and (30) the time-independence of the coefficients in the auxiliary equation would require now a time dependent coupling $g(t)=g_0b(t)$; in the Thomas-Fermi regime and with g constant, all coefficients become time independent with

$$\ddot{b}+\omega(t)^2b=\frac{\omega_0^2}{b^4},\qquad \tau(t)=\int_0^t\frac{dt'}{b(t')^3}. \tag{41}$$

In this case the boundary condition for $b(t_f)$ in (33) is modified to $b(t_f)=(\omega_0/\omega_f)^{2/5}$, assuming again $\ddot{b}(0)=\ddot{b}(t_f)=0$.

3.3 Remarks

Note that for a fixed g (for 2D, or the TF regimes in 1D and 3D), the non-linearity does not play any role in the design of optimal (frictionless) frequency trajectories since they only depend on the initial and final frequencies, the available time t_f and the functional form chosen for $b(t)$.

An important remark on the TF approximation used for 1D and 3D geometries is that the non-linear coupling cannot be arbitrarily strong. The condition $g|\Psi|^2/(\hbar\omega_0)\gg 1$ should be compatible with the derivation of the 1D GP equation [38] in a weak interaction limit, i.e., $a_s|\psi|^2\ll 1$, a_s being the s-wave scattering length.

As an alternative to the steps given after Eq. (29), we may impose that the coefficient multiplying $\rho^2 b^4\Psi$ must vanish instead of becoming a non-zero constant [41–43]. This amounts to imposing $\ddot{b}+\omega(t)^2 b=0$ instead of the Ermakov equation (5). Proceeding as in Sec. 3.1 with τ given by Eq. (30), the resulting auxiliary equation becomes

$$i\hbar\frac{\partial\Psi}{\partial\tau}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial\rho^2}+gb|\Psi|^2\Psi. \tag{42}$$

This is not an equation for the harmonic oscillator but for a condensate without confining external fields and with a, generically, time dependent non-linear coupling factor. If $g(t)=g_0/b(t)$ this method provides, from known analytical solutions of Eq. (42) with a constant factor $g(t)b(t)=g_0$, explicit solutions that have been used in the field of soliton dynamics [41–43]. The solutions $\psi(x,t)$ for the same $\omega(t)$ and initial conditions should of course be equivalent to the ones obtained with the ordinary Ermakov equation, but the later is better suited for the application of our inverse technique.

4 Comparison with the "transitionless tracking" (TT) algorithm

A different shortcut to adiabaticity is provided by the transitionless-tracking method [19]. Assume a time-dependent Hamiltonian $H_0(t)$ with initial and final values, instantaneous eigenvectors $|n(t)\rangle$ and eigenvalues $E_n(t)$,

$$H_0(t)|n(t)\rangle=E_n(t)|n(t)\rangle. \tag{43}$$

A slow change would preserve the eigenvalue and eigenvector along the dynamical evolution times a phase factor,

$$|\psi_n(t)\rangle=\exp\left\{-\frac{i}{\hbar}\int_0^t dt' E_n(t')-\int_0^t dt'\langle n(t')|\partial_{t'}n(t')\rangle\right\}|n(t)\rangle. \tag{44}$$

The populations are also preserved in a finite time by means of the following Hamiltonian $H(t)$ (which is denoted as H_{TT} if distinction with the other method is needed)

$$H(t)=\sum_n|n\rangle E_n\langle n|+i\hbar\sum_n\Big(|\partial_t n\rangle\langle n|-\langle n|\partial_t n\rangle|n\rangle\langle n|\Big)\equiv H_0+H_1. \tag{45}$$

The adiabatic approximation $[|\psi_n(t)\rangle$ for $H_0(t)$ represents the *exact* dynamics with $H(t)$,

$$i\hbar\partial_t|\psi_n(t)\rangle=H(t)|\psi_n(t)\rangle$$

with the simplified notation, $|n\rangle = |n(t)\rangle$. It is also possible to choose other phases in (44) [1]. The simplest case is $U(t) = \sum |n(t)\rangle\langle n(0)|$, without phase factors, corresponding to $H(t) = i\hbar \sum |\partial_t n\rangle\langle n|$. With this choice $H_0(t)$ has been formally suppressed in $H(t)$ but still plays a role through its eigenfunctions $|n(t)\rangle$.

For the harmonic oscillator

$$H_0(t) = \frac{1}{2m}\hat{p}^2 + \frac{1}{2m}\omega(t)^2\hat{x}^2 = \hbar\omega(t)\left(\hat{a}_t^\dagger \hat{a}_t + \frac{1}{2}\right), \tag{46}$$

where $\hat{a}_t$ and $\hat{a}_t^+$ are the Schrödinger-picture annihilation and creation operators at time t and are y the following form

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega(t)}}(a_t^\dagger + a_t), \tag{47}$$

$$\hat{p} = i\sqrt{\frac{\hbar m\omega(t)}{2}}(a_t^\dagger - a_t), \tag{48}$$

$$\hat{a}_t = \sqrt{\frac{m\omega(t)}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega(t)}\hat{p}\right), \tag{49}$$

$$\hat{a}_t^\dagger = \sqrt{\frac{m\omega(t)}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega(t)}\hat{p}\right). \tag{50}$$

Notice that the "instantaneous" ladder operators $\hat{a}_t$, $\hat{a}_t^\dagger$ create or annihilate different "instantaneous" states, adapted to the corresponding frequency. Ladder operators with different time labels do not commute in general, although some combinations, e.g., those equivalent to powers of $\hat{x}$ and/or $\hat{p}$, do commute, see below.

We find, using the recursion relation of Hermite polynomials and their orthogonality,

$$H_1(t) = i\hbar\frac{\dot{\omega}}{\omega(t)}\sum_n \left[\left(\frac{1}{4} - \frac{m\omega(t)}{2\hbar}\hat{x}^2\right)|n\rangle\langle n| + \sqrt{\frac{m\omega(t)}{2\hbar}}\hat{x}\sqrt{n}|n-1\rangle\langle n|\right]. \tag{51}$$

Using $a_t = \sum_n \sqrt{n}|n-1(t)\rangle\langle n(t)|$, $[\hat{x},\hat{p}] = i\hbar$,and the relations between $\hat{x}$, $\hat{p}$, $\hat{a}_t$ and $\hat{a}_t^\dagger$ written above, we may finally write the Hamiltonian $H_1(t)$ in the following forms

$$H_1(t) = -\frac{\dot{\omega}}{4\omega}(\hat{x}\hat{p} + \hat{p}\hat{x}) = i\hbar\frac{\dot{\omega}}{4\omega}\left(\hat{a}^2 - (\hat{a}^\dagger)^2\right). \tag{52}$$

The subscript t in $\hat{a}$ and $\hat{a}^\dagger$ has been dropped because the squeezing combination $\hat{a}^2 - (\hat{a}^\dagger)^2$ is independent of time, so it may be evaluated at any convenient time, e.g. at $t = 0$. The connection with squeezing operators is worked out in the appendix of Ref. [44].

The final Hamiltonian $H = H_0 + H_1$ is still quadratic in $\hat{x}$ and $\hat{p}$, so it may be considered a generalized harmonic oscillator [45], but the potential is a non-local operator. This is the main drawback for its physical implementation and its physical realizability remains

an open question. The II method is thus clearly distinct from from TT and implements a different Hamiltonian. Note also, by comparison of the coefficients, that the invariant operator I corresponding to H_{II} is different from H_{TT}, although they are both generalized harmonic oscillators.

5 Conclusions

In summary, the "inverse-invariant" method is able to cool down atoms in a harmonic trap without phase-space compression as in a perfectly slow adiabatic expansion but in a much shorter time by a special design of the time dependence of the frequency. For very short total expansion times this may require that the harmonic trap becomes transitorily an expulsive parabolic potential. It is also possible to take a Bose-Einstein condensate in a very short time from an initial harmonic trap to a final one without excitations, by the same technique. We have discussed advantages with respect to other methods: adiabatic processes, bang-bang techniques, and "transitionless-tracking" methods. As an outlook, similar techniques may inspire a way out to carry out adiabatic computation in a finite time [7,8], may be applied to the control of soliton dynamics of Bose-Einstein condensates [31, 46], pulsed beams [47], or in combination with transport of ultracold atoms or ions [48]. Fast driven expansions may also offer an enlarged and faithful copy of the initial system that can be imaged on much shorter times than with the standard time-of-flight technique based on free expansions.

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