Fast driving between arbitrary states of a quantum particle by trap deformation

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By performing a slow adiabatic change between two traps of a quantum particle, it is possible to transform an eigenstate of the original trap into the corresponding eigenstate of the final trap. If no level crossings are involved, the process can be made faster than adiabatic by setting first the interpolated evolution of the wave function from its initial to its final form and inferring from this evolution the trap deformation. We find a simple and compact formula which gives the trap shape at any time for any interpolation scheme. It is applicable even in complicated scenarios where there is no adiabatic process for the desired state transformation, e.g., if the state changes its topological properties. We illustrate its use for the expansion of a harmonic trap, for the transformation of a harmonic trap into a linear trap and into an arbitrary number of traps of a periodic structure. Finally, we study the creation of a node exemplified by the passage from the ground state to the first excited state of a harmonic oscillator.

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I. INTRODUCTION

There is a growing interest in accelerating transformations among different quantum states to limit the detrimental effect of decoherence or noise, or to increase the repetition rate, or the number of quantum operations that can be carried out in a given time interval [1]. A few methods that bypass adiabatic transformations by designing appropriate time-dependent Hamiltonians have been set up. This includes methods based on exact solutions with time-dependent scaling parameters [2–5], methods based on dynamical Lewis-Riesenfeld invariants [3,6,7], the transitionless tracking algorithm that adds counteradiabatic terms to the Hamiltonian [8–10], the fast-forward approach [11–18], Lie-algebraic methods [19,20], or the fast quasiadiabatic approach [21].

Recent experimental progress enables one to shape atomic traps dynamically using for instance lasers diffracted by spatial light modulators (see, e.g., [22]), time-dependent microwave dressing [23], or, for ions in multisegmented Paul traps, time-dependent voltages applied to the control electrodes [24]. Such trap shaping on a short time scale has been proven useful, for example, to implement quantum thermodynamical cycles [25,26], or to implement a scalable architecture for quantum information processing [27]. It is also important for some quantum information processing schemes such as multiplexing and demultiplexing when information is encoded in external degrees of freedom [7], for Fock state creation [28], or velocity control [29,30], and it is expected to become more and more relevant given the current interest to develop quantum technologies.

In this paper, we design the fast driving of a wave packet for a particle in a time and position-dependent trap potential with the aim of reaching some target state. We provide an explicit formal solution for the time-dependent potential that connects eigenstates of different traps, or different eigenstates of the same trap. The theoretical framework developed here builds on, and improves, the one presented in [13,14], where a streamlined version of the fast-forward method of Masuda and Nakamura [11,12] was derived and exemplified to drive a matter wave from a single well to a symmetric double well. The solution presented here reduces considerably the numerical time necessary to generate the appropriate time-dependent potential, and offers therefore the possibility to explore more complex state transformations. It also enables us to drive transitions that could not be handled with the techniques in [13,14], specifically transformations that change the topology of the state with the creation of a node.

In Sec. II we introduce the theoretical framework and explain the inverse protocol procedure. Section III presents several examples including ground-state to ground-state and first excited to first excited transformations, matter wave splitting in an arbitrary number of traps, and the transformation between states with different topology. In Sec. IV we discuss the results and open questions. Finally, the Appendix explains the procedure followed to make the quantities dimensionless.

II. FROM THE WAVE FUNCTION TO THE POTENTIAL

To drive a wave function from an eigenstate of an initial potential to an eigenstate of a final potential (which might be identical to the original one), we use a similar approach to the one in [13,14]. In this approach, the initial wave function, $\psi_{\rm i}(x)$, and final (target) wave function, $\psi_{\rm f}(x)$, are given. The wave function should evolve between these two states in a predetermined time $t_{\rm f}$, satisfying the boundary conditions $\psi(x,0)=\psi_{\rm i}(x)$ and $\psi(x,t_{\rm f})=\psi_{\rm f}(x)$. The corresponding time-dependent potential can in principle be deduced from the Schrödinger equation:

$$V(x,t)=\frac{1}{\psi(x,t)}\left(i\hbar\frac{\partial\psi(x,t)}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}\right). \quad (1)$$

Using the modulus-phase representation for the time-dependent wave function,

$$\psi(x,t)=\rho(x,t)e^{i\phi(x,t)}, \quad (2)$$

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the expression for the potential can be worked out, which in general becomes a complex function with real and imaginary parts. By imposing that the potential takes real values, $\mathrm{Im}[V(x,t)]=0$, we get a first relation that links the phase $\phi(x,t)$ and the modulus $\rho(x,t)$:

$$\frac{1}{\rho}\frac{\partial\rho}{\partial t}+\frac{\hbar}{2m}\left(\frac{2}{\rho}\frac{\partial\phi}{\partial x}\frac{\partial\rho}{\partial x}+\frac{\partial^2\phi}{\partial x^2}\right)=0. \tag{3}$$

This is a continuity equation. The expression for the potential then reads

$$V(x,t)=-\hbar\frac{\partial\phi}{\partial t}+\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial^2\rho}{\partial x^2}-\left(\frac{\partial\phi}{\partial x}\right)^2\right]. \tag{4}$$

Equation (3) can be integrated formally,

$$\frac{\partial\phi}{\partial x}=-\frac{mu(x,t)}{\hbar}, \tag{5}$$

where u plays the role of a "hydrodynamic velocity":

$$u(x,t)=\frac{1}{\rho^2(x,t)}\frac{\partial}{\partial t}\left(\int_0^x\rho^2(x',t)dx'\right). \tag{6}$$

The potential $V(x,t)$ can therefore be inferred from $\rho(x,t)$,

$$V(x,t)=m\frac{\partial}{\partial t}\int_0^x u(x',t)dx'+\frac{\hbar^2}{2m}\frac{1}{\rho(x,t)}\frac{\partial^2\rho(x,t)}{\partial x^2}-\frac{1}{2}mu^2(x,t)-\hbar\dot{\phi}_0(t), \tag{7}$$

where $\phi_0\equiv\phi(x=0,t)$ and the dot means time derivative. This is our central result.

In a previous streamlined version of the fast-forward approach [13,14], $\rho(x,t)$ was designed first and then the equation for the phase had to be solved numerically in order to get the potential. However, in the current improved formulation the potential only depends on $\rho(x,t)$, so we find it directly from Eq. (7). This is a great advantage because the computation time necessary to generate $V(x,t)$ is reduced considerably. Furthermore, as we will see in the examples, by reinterpreting the modulus and phase decomposition we can also solve more complicated problems.

Consider a transformation from the ground state, $\psi_\mathrm{i}(x)$, of a potential $V(x,0)$, to the ground state, $\psi_\mathrm{f}(x)$, of another potential, $V(x,t_\mathrm{f})$ in a time t_f. We may use the interpolation formula

$$\rho(x,t)=\mathcal{N}(t)\{[1-\eta(t)]\rho_\mathrm{i}(x)+\eta(t)\rho_\mathrm{f}(x)\}, \tag{8}$$

where $\rho_\mathrm{i}(x)=|\psi_\mathrm{i}(x)|$ and $\rho_\mathrm{f}(x)=|\psi_\mathrm{f}(x)|$, $\eta(t)$ is a monotonous and smooth function that varies from $\eta(0)=0$ to $\eta(t_\mathrm{f})=1$, and $\mathcal{N}(t)$ is a normalization factor. As the wave functions are ground states they have no nodes and the quantity $\rho(x,t)$ never vanishes. This ensures the absence of any divergent behavior in the potential (7). Furthermore, $\rho(x,t)$ in Eq. (8) is positive during the whole process by construction.

Assuming the boundary conditions

$$\begin{aligned}\dot{\eta}(0)&=\dot{\eta}(t_\mathrm{f})=0,\\ \ddot{\eta}(0)&=\ddot{\eta}(t_\mathrm{f})=0,\end{aligned} \tag{9}$$

we find from Eqs. (6) and (8)

$$\begin{aligned}\dot{\rho}(x,0)&=\dot{\rho}(x,t_f)=0,\\ u(x,0)&=u(x,t_f)=0,\end{aligned} \tag{10}$$

and consequently

$$\begin{aligned}V(x,0)&=-\hbar\dot{\phi}_0(0)+\frac{\hbar^2}{2m}\frac{1}{\psi_\mathrm{i}(x)}\frac{\partial^2\psi_\mathrm{i}}{\partial x^2},\\ V(x,t_\mathrm{f})&=-\hbar\dot{\phi}_0(t_\mathrm{f})+\frac{\hbar^2}{2m}\frac{1}{\psi_\mathrm{f}(x)}\frac{\partial^2\psi_\mathrm{f}}{\partial x^2}.\end{aligned} \tag{11}$$

To adjust the zero of the potential, we shall set $\dot{\phi}_0(0)=-E_\mathrm{i}/\hbar$ and $\dot{\phi}_0(t_\mathrm{f})=-E_\mathrm{f}/\hbar$, where E_i is the energy of the initial state and E_f is the one of the final state, and use an interpolation formula for $\phi_0(t)$ with the extra boundary conditions $\phi_0(0)=\phi_0(t_\mathrm{f})=0$ for simplicity.[1] For example, polynomial interpolations satisfying the boundary conditions for $\eta(t)$ and $\phi_0(t)$ are

$$\eta(t)=\frac{t^3}{t_\mathrm{f}^3}\left[1+3\left(1-\frac{t}{t_\mathrm{f}}\right)+6\left(1-\frac{t}{t_\mathrm{f}}\right)^2\right], \tag{12}$$

$$\phi_0(t)=\frac{t}{t_\mathrm{f}}\left(1-\frac{t}{t_\mathrm{f}}\right)\left[\frac{(E_\mathrm{i}+E_\mathrm{f})t-E_\mathrm{i}t_\mathrm{f}}{\hbar}\right]. \tag{13}$$

Note that due to Eqs. (5), (10), and (13) the phase $\phi(x,t)$ is zero at initial and final times.

III. EXAMPLES

A. Connecting ground states

We consider the transformation in a time t_f from the ground-state wave function of a one-dimensional harmonic potential of angular frequency ω_i to the ground state of a harmonic potential of angular frequency $\omega_\mathrm{f}=\xi\omega_i$. For $\xi<1$ ($\xi>1$), this transformation corresponds to an expansion (compression). Such a transformation can be carried out in a long time using an adiabatic evolution. Our fast inverse protocol amounts to bypassing the adiabatic evolution.

From now on we consider dimensionless quantities. The initial wave function and the final one in dimensionless units (with $\hbar=m=\omega_\mathrm{i}=1$; see the Appendix for more details) read

$$\begin{aligned}\psi_\mathrm{i}(x)&=\pi^{-1/4}e^{-x^2/2},\\ \psi_\mathrm{f}(x)&=\xi^{1/4}\psi_\mathrm{i}(x\sqrt{\xi}).\end{aligned} \tag{14}$$

The explicit form for $\mathcal{N}(t)$ and $\rho(x,t)$ can be readily worked out from Eqs. (8) and (12). In Fig. 1(a), we provide an example of fast time evolution of the potential $V(x,t)$ from Eq. (7), with $\xi=1/3$ and $t_\mathrm{f}=0.24\times2\pi$. Note that the transformation is here performed on a time scale significantly smaller than the final period. The curvature of the potential becomes transiently negative at the center of the trap (from $t=t_\mathrm{f}/8$ to $3t_\mathrm{f}/5$) in order to speed up the transformation [3,4].

[1] Alternatively, we can set the initial and final energy to zero, imposing $\phi_0(t)=0$. This simply amounts to a "vertical" shift of the potential with respect to the polynomial interpolation in Eq. (13). In this paper we use the polynomial form in Eq. (13).

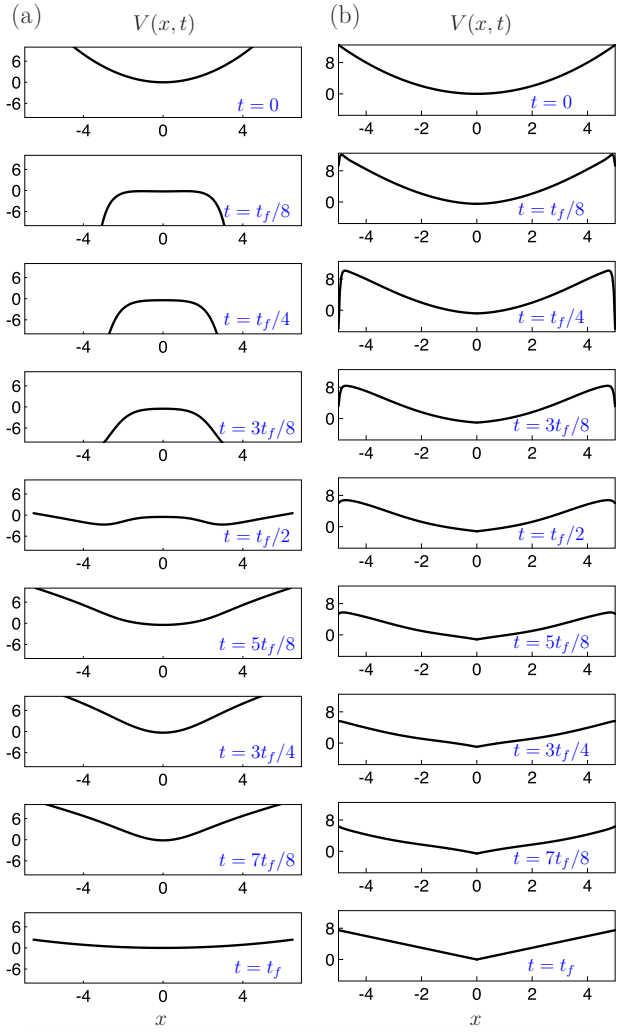

FIG. 1. (a) Snapshots of the time evolution of the trap shape from a harmonic potential of initial angular frequency 1 to a harmonic potential of final angular frequency $1/3$ that guarantees the perfect transfer of the ground state of the initial trap to that of the final trap in a short time $t_f = 0.24 \times 2\pi$. (b) Snapshots of time evolution of the trap shape from a harmonic potential $U_H(x) = x^2/2$ to a linear trap $U_L(x) = 3|x|/2$ in a time interval $t_f = 0.24 \times 2\pi$ that ensure the perfect transfer of the ground state of the initial trap to that of the final trap.

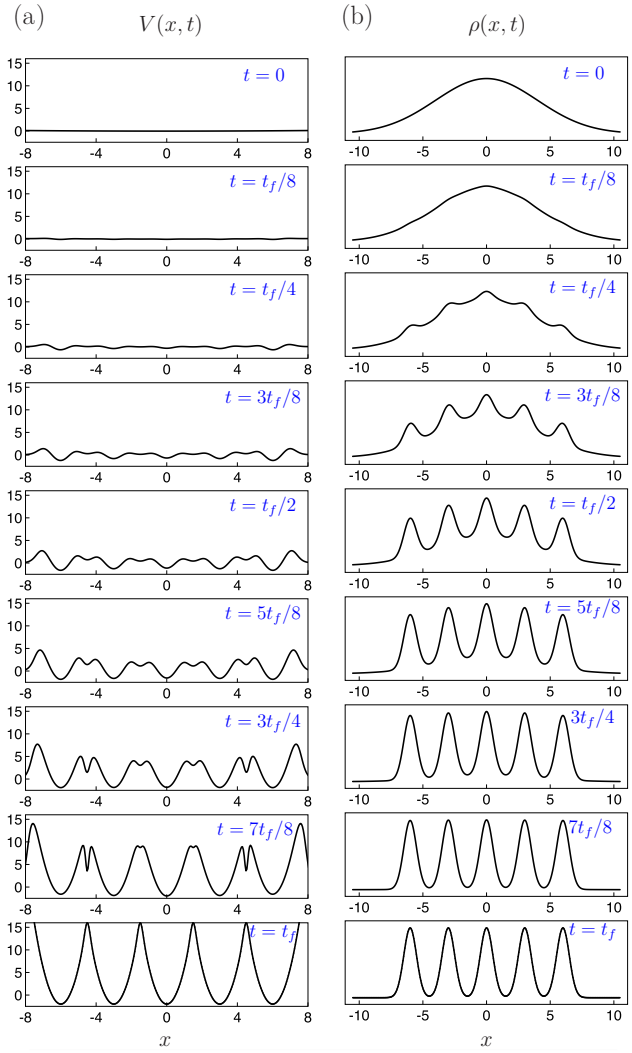

FIG. 2. (a) Snapshots of the time evolution of the trap shape that splits the wave function of a harmonic potential (of angular frequency $\omega_0 = 1$) in five equidistant wave functions with the same weight. The transformation is performed in a time $t_f = 10\pi$. (b) Snapshots of $\rho(x,t)$ (arbitrary units) vs position in the course of the transformation.

For this expansion operation we may compare the current method with the polynomial solution of the invariant-based method presented in [3]. Given the same initial and final angular frequencies, $\omega_i = 1$ and $\omega_f = 1/3$, the operation times necessary to keep the frequency real during the whole process are $t_f \geqslant 0.365 \times 2\pi$ in the invariant-based method, and $t_f \geqslant 0.32 \times 2\pi$ in the current approach. Further advantages of the method developed in this paper will be demonstrated in later examples, for which other approaches cannot be implemented. For example, the invariant-based method may be limited by the difficulty of finding a simple invariant of the system, or difficulties to change the topology of the state [13] when using a coordinate representation (invariants were used for that end in [7], but within a two-level approximation).

The method developed here also gives the potential to connect two ground states of traps of different kind. This is illustrated in Fig. 1(b). The ground state of a harmonic potential $U_H(x) = x^2/2$ is transformed into the ground state of a linear potential $U_L(x) = 3|x|/2$ in a time interval $t_f = 0.24 \times 2\pi$.

B. Splitting of a wave function

The invariant-based method and the transitionless tracking approach are problematic for splitting wave functions [13,14]. This is to be contrasted with the simplified fast-forward method [13,14]. The compact formula (7) allows us, for example, to split the wave function into an arbitrary number of parts. In Fig. 2 the ground-state wave function, $\psi_i(x)$, of a harmonic potential of angular frequency ω_0 is split into five parts (given by ground states of corresponding harmonic oscillators) separated by a distance of $3a_0/4 = 3(\hbar/m\omega_0)^{1/2}/4$, each having an eighth of the initial width. The time-dependent

potential deduced from the theoretical framework provides an exact solution for the perfect loading of a periodic structure, an important operation for cold atoms [15,31–35]. The transformation is performed here in a time interval equal to 10π for $\omega_0 = 1$.

C. Connecting first excited states

The approach presented in Sec. II can be readily generalized to transform the first excited state of a given trap into the first excited state of another trap in a short time. From Eqs. (5) and (10) and the boundary conditions $\phi_0(0) = \phi_0(t_f) = 0$, the condition for the phase $\phi(x,0) = \phi(x,t_f) = 0$ is fulfilled by construction. Thus, a way to define an odd state using Eq. (2) is to assume that $\rho(x,t)$ may take negative values. The ansatz in Eq. (8) generates a positive $\rho(x,t)$ so we set a new one:

$$\rho(x,t) = \mathcal{N}(t)\{[1-\eta(t)]\psi_i(x) + \eta(t)\psi_f(x)\}. \tag{15}$$

For the transformation between two harmonic traps considered in Sec. III A ($\omega_i = 1, \omega_f = 1/3$), Fig. 3(a) shows the evolution of $V(x,t)$ using Eq. (7) and Eqs. (12), (13), and (15). In Fig. 3(b) $\rho(x,t)$ is represented. The process time is $t_f = 0.48 \times 2\pi$.

D. Connecting ground and first excited states

The connection between states with different topological properties is of much interest for quantum computing processes because it allows one, for example, to prepare Fock states by deforming the trap without using laser excitation of internal states [7]. Using sequences of π pulses is demanding, as creating N-phonon Fock states needs very precise N pulses, but fluctuations in intensity, frequency, and timing imperfections give a reduced fidelity [36].

We want to drive the system from an even state (ground) to an odd one (first excited) of the harmonic oscillator with frequency $\omega_0/(2\pi)$. This was left as an open question in [13]. Whenever $\rho(x,t)$ has a definite symmetry (even or odd with respect to $x = 0$), the potential in Eq. (7) will have even symmetry. The reason lies in Eq. (6), since for an either even or odd $\rho(x,t)$, the "hydrodynamic velocity" $u(x,t)$ is always odd. Thus the potential becomes a sum of even functions and stays even throughout the process. Therefore, the parity of the initial state will be preserved, and using the interpolation in Eq. (8) for $\rho(x,t)$ the system cannot be driven from the even initial state to the desired odd final state. Note in addition the numerical difficulties because of the discontinuity of $\partial_x \rho(x,t)$ at zeros of $\rho(x,t)$.

The connection will be achieved by allowing $\rho(x,t)$ to be asymmetric so that the potential in Eq. (7) becomes in general a sum of even and odd functions. The use of Eq. (15) as the interpolation formula is a simple way to get an asymmetric $\rho(x,t)$. The potential is singular when $\rho(x,t) = 0$ but, as we will see, these are mild singularities in the sense that they may be numerically handled by truncation. The singularity begins at $x \to -\infty$ when $t \to 0$ and moves to the right. At t_f the singularity ends up at the center ($x = 0$) and it is canceled by the zero of $\partial_x^2 \rho(x,t)$ there.

An alternative way to design the interpolation of $\rho(x,t)$ would be, instead of using Eqs. (8) and (15), to design $\rho(x,t)$ directly from the wave function as a positive square root of the density:

$$\rho(x,t) = \sqrt{|\psi(x,t)|^2}. \tag{16}$$

We have unsuccessfully tested this ansatz trying different interpolations for $\psi(x,t)$. Choosing the interpolating wave function in the form $\psi(x,t) = \mathcal{N}[(1-\eta)\psi_i + i\eta\psi_f]$ and substituting in Eq. (16), the modulus, $\rho(x,t) = |\mathcal{N}|((1-\eta)^2|\psi_i|^2 + \eta^2|\psi_f|^2)^{1/2}$, vanishes only at the boundary of the time interval, but the resulting $\rho(x,t)$ has a definite even symmetry. We have also tried the interpolation $\psi(x,t) = N(t)\{[1-\eta(t)]\psi_i(x) + \eta(t)\psi_f(x)\}$, which, substituted in Eq. (16), generates an asymmetric function. However, the desired final state could not be reached numerically due to singularities that affect the successive derivatives of $\rho(x,t)$,

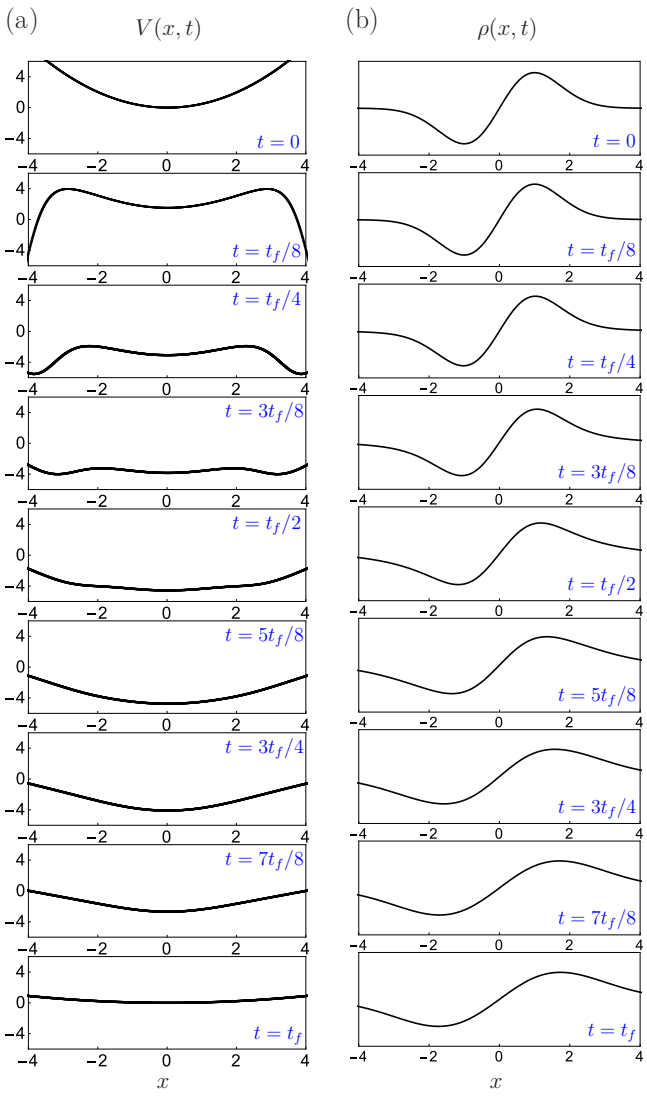

FIG. 3. (a) Snapshots of the time evolution of the trap shape from a harmonic potential of initial angular frequency $\omega_i = 1$ to a harmonic potential of final angular frequency $\omega_f = 1/3$ that ensures the perfect transfer of the first excited state of the initial trap to that of the final trap in a short time $t_f = 0.48 \times 2\pi$. (b) Snapshots of the time evolution of the corresponding $\rho(x,t)$ (in arbitrary units).

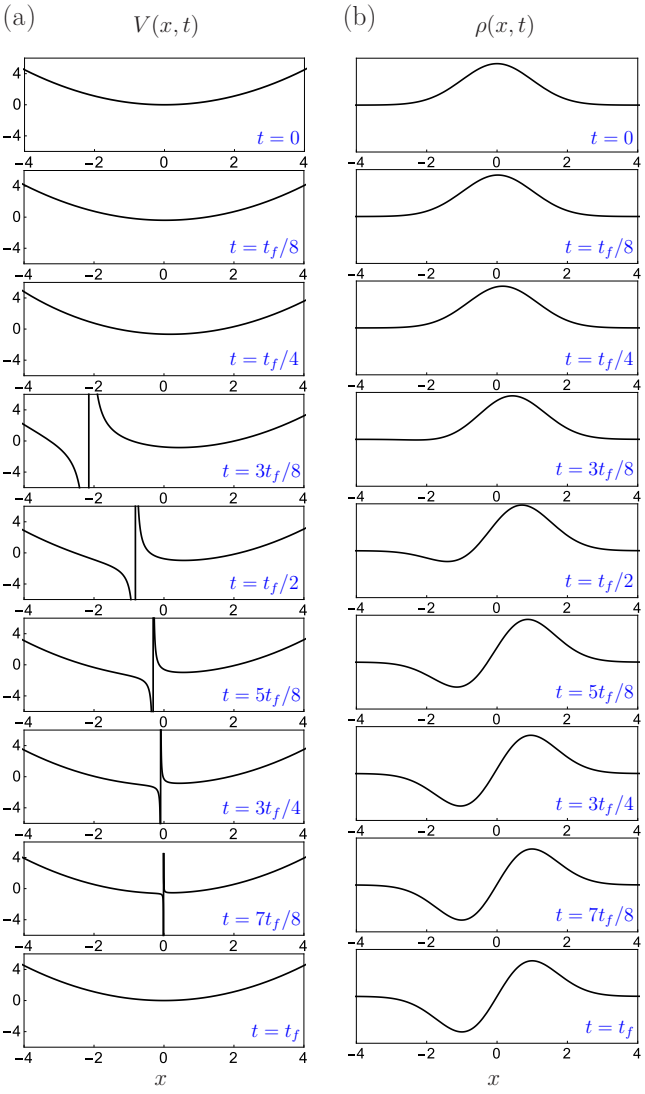

FIG. 4. (a) Snapshots of the time evolution of the trap shape that connects the ground state to the first excited state of a harmonic potential ($\omega_0 = 1$). The transformation is calculated in a time $t_f = 8\pi$. (b) $\rho(x,t)$ (in arbitrary units) is plotted as a function of the position in the course of the transformation.

because of the definition of $\rho(x,t)$ via a modulus. Therefore, hereinafter we will use the protocol in Eq. (15) to connect the ground and first excited states.

Imposing that the initial and final states ($\hbar = m = \omega_0 = 1$) are

$$\psi_i(x) = \pi^{-1/4} e^{-x^2/2}, \qquad \psi_f(x) = \pi^{-1/4} x\sqrt{2} e^{-x^2/2}, \tag{17}$$

and substituting in Eq. (15), we get the explicit form of the wave amplitude:

$$\rho(x,t) = \pi^{-1/4} \frac{1 + [x\sqrt{2} - 1]\eta(t)}{\sqrt{1 + 2[\eta(t) - 1]\eta(t)}} e^{-x^2/2}. \tag{18}$$

Using Eqs. (12), (13), and (18) in Eq. (7), we find the potential evolution represented in Fig. 4(a). Figure 4(b) shows the evolution of $\rho(x,t)$ given by Eq. (18). The system may thus be driven from the ground state into the first excited state without final excitations in a finite, arbitrarily short time.

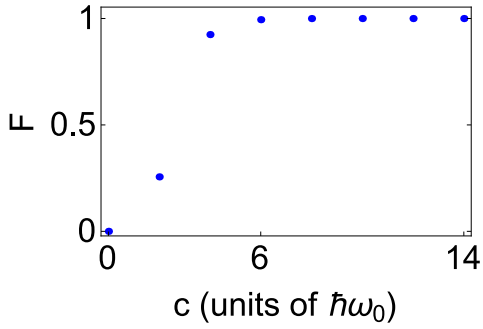

FIG. 5. Fidelity $F \equiv |\langle \psi^e(x,t_f)|\psi_f(x)\rangle|^2$ vs the potential truncation constant c, where $\psi^e(x,t_f)$ is the final wave function evolved using the truncated potential V_{trun}. $t_f = 8\pi/\omega_0$.

The effect of the divergence of the potential at a position for intermediate times [see Fig. 4(a)] is now studied by truncating the potential as

$$V_{\text{trun}}(x,t) = \begin{cases} V(x,t) & \text{if} \quad -c < V(x,t) < c \\ c & \text{if} \quad V(x,t) \geqslant c \\ -c & \text{if} \quad V(x,t) \leqslant -c \end{cases}, \tag{19}$$

where c is a positive real number. To check the stability of the method under this approximation, we compute the fidelity between the final state ψ_f and the final state evolved by the truncated potential $\psi^e(x,t_f)$ for different values of c. The evolution of $\psi^e(x,t_f)$ is calculated using the "split-operator method" with the truncated Hamiltonian $H_{\text{trun}} = T + V_{\text{trun}}$, T being the kinetic energy. Figure 5 shows that the method is stable for large enough c. For a relative small value of $c = 8\hbar\omega_0$ the transition is performed with a 0.9996 fidelity.

IV. CONCLUSION

We have proposed an improved version of the fast-forward approach described in [13,14]. In this formalism, the solution of the time-dependent potential is explicit, reducing the computational time. We applied this technique to accelerate some basic operations that are relevant for quantum information processing and fundamental studies, such as expansions or compressions of a harmonic trap, splitting of a wave function, and generic driving between eigenstates. In particular, we have dynamically transformed the ground state into the first excited state of a harmonic potential. The connection has been realized allowing the wave amplitude $\rho(x,t)$ to be asymmetric and take negative values. The approach in [7] was based on a two level approximation that breaks down for fast processes. In comparison, the current approach can in principle be applied to shorter times, limited by the technical abilities to implement time-dependent nontrivial potentials, which are progressing quite rapidly [22]. Furthermore, the fast-forward protocol may also be used to create higher Fock states just by changing the final states.

An open question left for future work is to optimize the robustness versus noise and perturbations [6]. In addition, it

would also be interesting to apply the method developed here to infinite square wells in order to study "exotic quantum holonomy" transformations [37]. Applications of the method can go beyond quantum mechanics, e.g., to determine potentials in a Fokker-Planck equation [38].

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APPENDIX: DIMENSIONLESS FORMULATION

Here we explain the procedure followed to make the quantities in Sec. III dimensionless. Starting from the one-dimensional time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\psi(x,t), \qquad \text{(A1)}$$

we define the inverse of the angular frequency $\omega_{\rm i}$ as the unit of time, m as the unit of mass, $\hbar\omega_{\rm i}$ as the unit of energy, and $a_0 = \sqrt{\hbar/(m\omega_{\rm i})}$ as the unit of length. The dimensionless quantities (defined by now with a tilde) are

$$\begin{aligned}
\tilde{\hbar} &= \frac{\hbar\omega_{\rm i}}{\hbar\omega_{\rm i}} = 1,\\
\tilde{\omega}_{\rm i} &= \frac{\omega_{\rm i}}{\omega_{\rm i}} = 1,\\
\tilde{m} &= \frac{m}{m} = 1,\\
\tilde{t} &= \omega_{\rm i} t,\\
\tilde{E} &= \frac{E}{\hbar\omega_{\rm i}},\\
\tilde{x} &= \frac{x}{a_0},\\
\tilde{\psi}(x,t) &= \sqrt{a_0}\,\psi(x,t). \qquad \text{(A2)}
\end{aligned}$$

From Eqs. (A2) and (A1) we get the dimensionless Schrödinger equation

$$i\frac{\partial}{\partial\tilde{t}}\tilde{\psi}(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial\tilde{x}^2}\tilde{\psi}(x,t) + \tilde{V}(x,t)\tilde{\psi}(x,t), \qquad \text{(A3)}$$

which is the one used in Sec. III. However, in that section we remove the tildes, as it is customary to avoid a heavy notation, and simply set $\hbar = m = \omega_i = 1$. Also, notice that in the examples in which the angular frequency is constant the unit of time is ω_0^{-1}.

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