Coherent Atom Transport via Enhanced Shortcuts to Adiabaticity: Double-Well Optical Lattice

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Theoretical studies of coherent atom transport have as yet mainly been restricted to one-dimensional model systems with harmonic trapping potentials. Here we investigate this important phenomenon - a prerequisite for a variety of quantum-technology applications based on cold neutral atoms - under much more complex physical circumstances. More specifically, we study fast atomic transport in a moving double-well optical lattice, whose three-dimensional (anharmonic) potential is nonseparable in the $x - y$ plane. We first propose specific configurations of acousto-optic modulators that give rise to the moving-lattice effect in an arbitrary direction in this plane. We then determine moving-lattice trajectories that enable single-atom transport using two classes of quantum-control methods: shortcuts to adiabaticity (STA), here utilized in the form of inverse engineering based on a quadratic-in-momentum dynamical invariant of Lewis-Riesenfeld type, and their recently proposed modification termed enhanced STA (eSTA). Subsequently, we quantify the resulting single-atom dynamics by numerically solving the relevant time-dependent Schrödinger equations and compare the efficiency of STA- and eSTA-based transport by evaluating the respective fidelities. We show that - except for the regime of shallow lattices - the eSTA method consistently outperforms its STA counterpart. This study has direct implications for neutral-atom quantum computing based on collisional entangling two-qubit gates and quantum sensing of constant homogeneous forces via guided-atom interferometry.

I. INTRODUCTION

Fast, nearly lossless, transport of cold neutral atoms \cite{1,12} is of paramount interest for emerging quantum technologies \cite{12}, such as quantum sensing based on atom interferometry \cite{14,11} and neutral-atom quantum computing (QC) \cite{17,24}. It is also a prerequisite for analog simulation \cite{23} and quantum-state engineering in neutral-atom ensembles \cite{25,27}. In particular, coherent atom transport \cite{28} enabled by moving the confining optical trap – either an optical lattice or a tweezer \cite{29,30,42–44} – has attracted considerable attention quite recently, both theoretically and experimentally \cite{10,12,33,34}. While the renewed interest on the experimental side is largely interwoven with the recent progress pertaining to the scalability of optically-trapped neutral-atom systems \cite{35,36}, increased theoretical activity is motivated in part by the availability of a powerful family of control protocols based on STA \cite{37} and their recently proposed modification known as eSTA \cite{28,32}.

In single-atom transport one aims for a final atomic state that closely matches the initial one in the rest frame of the moving trap (up to an irrelevant global phase), which is equivalent to demanding minimization (or, in the ideal case, complete absence) of vibrational excitations at the end of transport. This last requirement, however, does not necessarily rule out the existence of transient excitations at intermediate times \cite{3}, a circumstance that motivates one to consider moving-trap trajectories using STA-based control protocols \cite{37}. Namely, STA protocols typically lead to the same final states as their adiabatic counterparts, but require significantly shorter times to accomplish that. This, in turn, alleviates the debilitating effects of noise and decoherence. Given that adiabatic changes of control parameters typically leave some dynamical properties of the system invariant, inverse-engineering techniques based on Lewis-Riesenfeld invariants (LRIs) \cite{40} proved to be the most pervasive ones among STA methods.

Theoretical investigations of single-atom transport have as yet mostly been restricted to one-dimensional (1D) systems \cite{3,11} with purely harmonic confining potentials \cite{2,7}. Yet, such simplifications often do not apply in realistic systems; either there is a significant coupling between the longitudinal and transverse degrees of freedom or the relevant confining potential is anharmonic. To bridge the gap between realistic experimental features and state-of-the-art theoretical studies, we have quite recently addressed atom transport \cite{33} in moving optical lattices (conveyor belts) \cite{29,30,42,44} using both STA- and eSTA methods. Taking into account the full anharmonic, 3D optical potential of conveyor belts, we have demonstrated the superiority of the eSTA-based atom transport protocols compared to STA-based ones for all but the lowest optical-lattice depths \cite{33}.

Attempting to demonstrate the possibility of a time-efficient atom transport under even more complex physical circumstances, in this paper we investigate an optical lattice characterized by a nonseparable potential \cite{45}. More precisely, we study both STA- and eSTA-based single-atom transport in a moving double-well optical lattice (DWOL), a 3D system whose corresponding potential in the $x - y$ plane cannot be written as a sum of $x$- and $y$-dependent contributions \cite{46,47}. Initially introduced with the aim of realizing a controlled entanglement of atoms in isolated pairs \cite{48,50}, DWOLs have subsequently been proposed as a testbed for a number of interesting quantum-coherent phenomena with cold atoms.
Examples include metastable incommensurate superfluidity [51, 52], superfluid-to-Mott-insulator quantum phase transitions [53, 54], superfluid-drag phenomena [55], nonlinear looped band structure of Bose-Einstein condensates [56], to name but a few. The nontrivial geometrical structure of DWOLs gives rise to unconventional features in the single-particle energy spectrum. For instance, a parameter regime exists where the first excited Bloch band of a DWOL has degenerate energy minima at nonzero quasimomenta [57]. Such band minima at nonzero quasimomenta are quite a rare occurrence in other physical systems, where they typically do not have a purely kinetic origin but are instead brought about by the presence of interactions [57, 60].

We first propose specific configurations of acousto-optic modulators (AOMs) that give rise to the moving-lattice effect in an arbitrary direction in the $x-y$ plane of a DWOL. We subsequently model coherent atom transport using two classes of control protocols: STA-type ones, here obtained using inverse-engineering techniques based on LRI, as well as those originating from eSTA. Having determined the trajectories of the moving lattice using these two state-of-the-art methods, we compute the resulting single-atom dynamics by numerically solving the corresponding time-dependent Schrödinger equations using the Fourier split-operator method. Finally, we quantify and compare the efficiency of STA- and eSTA-based atomic transport by evaluating the corresponding fidelities for a broad range of values of the relevant parameters (lattice depths, transport distances, etc.).

We demonstrate that both STA and eSTA allow time-efficient atom transport in DWOLs. In particular, while STA provides somewhat faster transport in shallow lattices (i.e. for relatively low lattice depths), eSTA becomes superior to it for larger lattice depths. Our numerical calculations show that this superiority of eSTA approach compared to its STA counterpart is more pronounced for shorter transport distances. In other words, for larger transport distances one also needs larger lattice depths for eSTA-based atomic transport to be faster than its STA-based counterpart. This is an important conclusion from the methodological standpoint as – due to its heuristic character – the eSTA method cannot a priori be expected to consistently outperform STA.

The outline of the remainder of this paper is as follows. In Sec. II we first provide the basic background of the atom-transport problem, specifying the full Hamiltonian governing such transport in a DWOL and the relevant distance, time, and energy scales. We then introduce DWOLs, specifying first their full 3D optical potential and then proposing configurations of AOMs that enable single-atom transport in this system. In Sec. III we discuss the methodology for obtaining STA-based trajectories of a moving DWOL and present typical resulting trajectories. The following Sec. IV addresses the same problem using the eSTA method. In Sec. V after briefly introducing our chosen computational method (the Fourier split operator method) for evaluating single-atom dynamics, we describe the use of the same method in conjunction with the imaginary-time evolution approach for obtaining the ground state of the system. We then discuss the methodology for solving the time-dependent Schrödinger in the comoving reference frame, followed by the relevant details of our numerical implementation thereof. The results obtained for the atom-transport fidelity within both STA and eSTA methods are presented and discussed in Sec. VII. The quantum-technology implications of fast atom transport in DWOLs are discussed in detail in Sec. VIII. Before closing, we provide a short summary of the paper – along with the statement of the main conclusions drawn – in Sec. IX. Some cumbersome mathematical details are relegated to Appendices A, B, and C.

II. DWOL AND MOVING-LATTICE EFFECT

In the following, we will be concerned with the problem of transporting an atom of mass $m$ (e.g. of $^{87}Rb$) located at the time $t = 0$ in one of the lattice-potential minima of a DWOL, to another minimum at a distant location in the $x-y$ plane. In Sec. IIA below we briefly describe the background of this problem and introduce the relevant spatial, temporal, and energy scales. We then introduce the main features and characteristic parameters of DWOLs in Sec. IIB while in Sec. IIC we discuss specific configurations of AOMs in this system that give rise to the moving-lattice effect in different spatial directions.

A. Single-atom transport in DWOLs

In line with the conventional atom-transport phenomenology, the transport distance $d$ will be assumed in what follows to be at least an order of magnitude larger than the size $l_0$ of the atomic ground-state wave packet, i.e. $d \gtrsim 10 l_0$. The relevant Hamiltonian describing single-atom transport in the $x-y$ plane of a DWOL is given by

$$H_D(t) = -\frac{\hbar^2 \nabla^2}{2m} + U_D \left[ r - q_0(t) \right],$$

(1)

where $U_D(x,y,z)$ is the full optical potential of a DWOL (cf. Sec. IIA below) and $q_0(t) \equiv \{q_{0,x}(t), q_{0,y}(t), 0\}^T$ the time-dependent vector describing the moving-DWOL trajectory. In Secs. III and IV below we discuss the design of such trajectories using STA- and eSTA methods, respectively, that enable fast atomic transport in this system. While our approach – as emphasized in Sec. IIC – enables transport along an arbitrary direction in the $x-y$ plane, we will mostly be interested in the $x$, $y$, and diagonal directions. In what follows, the transport distances in these three directions will be denoted by $d_x$, $d_y$, and $d_z$, respectively.

To facilitate further discussion, we specify at this point the characteristic time-, length-, and energy scales in the
problem at hand. The oscillation periods \( T_x \equiv 2\pi/\omega_x \) and \( T_y \equiv 2\pi/\omega_y \) that correspond to the harmonic potential approximating the full DWOL optical potential [cf. Sec. 11B in the \( x \)- and \( y \)-directions will serve as the relevant time scales characterizing atom transport in the respective directions. At the same time, the corresponding harmonic-oscillator zero-point lengths \( l_x \equiv \sqrt{\hbar/(2m\omega_x)} \) and \( l_y \equiv \sqrt{\hbar/(2m\omega_y)} \) will serve as the characteristic lengthscales. Finally, all energies in the problem under consideration will be expressed in units of the recoil energy \( E_R^{} = \hbar^2 k_L^2/(2m) \), where \( k_L \) is the magnitude of the relevant laser wave vector \( k_L \).

It is worthwhile to mention that atom transport in DWOLs was investigated more than a decade ago using the idea of adjustable optical potentials in conjunction with optimal-control methods [61]. Yet, this previous study only considered atom transport between neighboring sites of a DWOL. In contrast to this previous study, our present approach is designed so as to facilitate coherent atom transport over an – in principle – arbitrary distance in the \( x-y \) plane of a DWOL. In addition, this approach is also based on a completely different physical mechanism (the moving-lattice effect enabled by AOMs) and entails different theoretical methodologies for designing specific transport trajectories (the STA and eSTA methods instead of the optimal-control techniques).

**B. DWOL: geometric structure and underlying optical potential**

The DWOL is constructed from two 2D lattices with different periods, thus its unit cell – whose orientation can be changed – contains two sites. Importantly, the height of the barrier between the two sites and their relative depth (“tilt”) are controllable. DWOLs entail a nonseparable optical double-well potential in the \( x-y \) plane and an independent, conventional optical potential in the \( z \)-direction that provides 3D confinement. In particular, the potential in the \( x-y \) plane consists of two components, which originate, respectively, from “in-plane”-polarized light (with intensity \( I_{xy} \)) and light polarized in the \( z \)-direction (with intensity \( I_z \)).

Using the general expression for the light intensity \( I \)

\[
I(x, y, z) = c|E(x, y, z)|^2, \tag{2}
\]

and adopting the paraxial approximation \( w_{0,x/y} \gg k_x^{-1} \) as well as the assumption that \( |z| \gg Z_R^{-1} \), one finds the total intensity in the form

\[
I_r(x, y, z)/I_{xy} = \cos^2 \left( \frac{\beta}{2} \right) \tilde{I}_{\|} + \sin^2 \left( \frac{\beta}{2} \right) \tilde{I}_1 + \xi_z \tilde{I}_z + \sqrt{\xi_z} \cos \left( \frac{\beta}{2} \right) \tilde{I}_{\perp}, \tag{3}
\]

Here \( I_{xy} \equiv 2 c|E_{xy}|^2 \), with \( E_{xy} \) being the electric-field amplitude of the lasers forming the 2D DWOL in the \( x-y \) plane. Different contributions to the total intensity in Eq. \( I_r \) are given by

\[
\tilde{I}_1 = \cos \left[ k_L \left(x + \frac{\pi}{2k_L}\right) - 2\theta_x - 2\phi_y \right] + \cos (2k_L y + 2\phi_y) + 2, \tag{4}
\]

\[
\tilde{I}_1 = 2 \left\{ \cos \left[ k_L \left(x + \frac{\pi}{2k_L}\right) - \theta_z - \phi_x \right] + \cos (k_L y + \phi_y) \right\}, \tag{5}
\]

\[
\tilde{I}_z = \frac{w_{0,x}w_{0,y}}{w_y(z)w_x(z)} \cos^2(k_z z) \times \exp \left( -2 \frac{x^2}{w^2_x(z)} + \frac{y^2}{w^2_y(z)} \right), \tag{6}
\]

\[
\tilde{I}_1 = 2 \sqrt{\frac{w_{0,x}w_{0,y}}{w_y(z)w_x(z)}} \exp \left( - \frac{x^2}{w^2_x(z)} + \frac{y^2}{w^2_y(z)} \right) \times \cos(k_z z) \sin \left( \frac{\phi}{2} \right) \tilde{E}_x^z + \cos \left( \frac{\phi}{2} \right) \tilde{E}_y^z. \tag{7}
\]

The \( z \)-dependent transverse beam waists \( w_u(z) (u = x, y) \) in Eqs. \( 3 \) and \( 7 \) are given by

\[
w_u(z) = w_{u,0} \sqrt{1 + \left( \frac{z}{Z_{R,u}} \right)^2}, \tag{8}
\]

with \( Z_{R,x} \) and \( Z_{R,y} \) being the respective Rayleigh lengths. At the same time, \( \tilde{E}_x^z = \tilde{E}_x^z/E_{xy} \) and \( \tilde{E}_y^z = \tilde{E}_y^z/E_{xy} \) in Eq. \( 7 \) stand for the dimensionless electric-field components in the \( x \)- and \( y \)-directions, respectively, corresponding to the \( x \)- and \( y \)-plane polarization:

\[
\tilde{E}_x^z = \exp (2i\phi_y) \exp \left[ -ik_L \left(x + \frac{\pi}{2k_L}\right) \right] \exp (2i\phi_y) \]

\[
\tilde{E}_y^z = \exp (i\phi_y) \left[ \cos (-ik_L y) + \exp (ik_L y) \exp (2i\phi_y) \right]. \tag{9}
\]

The angles \( \phi_x \) and \( \theta_x \) in Eqs. \( 4 \) and \( 5 \) correspond to phase-shifts and represent a remnant of generally polarization-dependent paths, as indicated by the subscripts \( r \) and \( z \) for path differences pertaining to the in- and out-of-plane light, respectively. These phases can most easily be understood from Fig. 3 below. While the angle \( \theta_x \) is due to the additional path that either the beam described by \( k_3 \) or the one denoted by \( k_4 \) needs to travel before passing through the origin again, the combination \( 2\phi_x + \phi_x \) corresponds to the phase-shift introduced due to the path difference between the the two incoming laser beams \( k_1 \) and \( k_2 \). This definition becomes clearer when comparing Fig. 3 with the general setup used for a static DWOL. In the latter case the wave-vector \( k_2 \) is not introduced separately to \( k_1 \) but rather as a result of an additional reflection of \( k_4 \) after passing through the origin.
Without loss of generality, we hereafter restrict our discussion to a DWOL oriented along the $x$ axis, which corresponds to the values $\phi_s = \phi_r = \theta_r = 0$ and $\theta \equiv \theta_z$ of the relevant parameters. The total DWOL potential in that case (for an illustration, see Fig. 1) is given by

$$U_D(x, y, z) = -U_{d,0} \left[ \tilde{U}_\parallel(x, y) + \tilde{U}_\perp(x, y) + \tilde{U}_z(x, y, z) + \tilde{U}_{cr}(x, y, z) \right], \quad (10)$$

where $U_{d,0} \equiv \alpha S_{xy} / (2c)$, with $\alpha S_{xy}$ being the polarizability corresponding to the scalar light shift [63], and different (dimensionless) contributions to this total potential are

$$\tilde{U}_\parallel = \cos^2 \left( \frac{\beta}{2} \right) \left[ \cos(2k_L y) - \cos(2k_L x) + 2 \right],$$

$$\tilde{U}_\perp = 2 \sin^2 \left( \frac{\beta}{2} \right) \left[ \cos(k_L y) - \sin(k_L x - \theta) \right]^2,$$

$$\tilde{U}_z = \xi_z \frac{w_{xy}^2 w_{xy}^2}{w_x(z) w_y(z)} \cos^2(k_x z) \times \exp \left( -2 \left[ \frac{x^2}{w_x^2(z)} + \frac{y^2}{w_y^2(z)} \right] \right), \quad (11)$$

$$\tilde{U}_{cr} = 2 \sqrt{\xi_z} \cos \left( \frac{\beta}{2} \right) \sqrt{\frac{w_{xy} w_{xy}}{w_x(z) w_y(z)}} \times \exp \left( - \left[ \frac{x^2}{w_x^2(z)} + \frac{y^2}{w_y^2(z)} \right] \right) \cos(k_x z) \times \left[ \cos \left( \frac{\phi}{2} \right) \cos(k_L y) - \sin \left( \frac{\phi}{2} \right) \sin(k_L x) \right].$$

In the above equations, $\xi_z \equiv I_z / I_{xy}$ is the relative intensity between the lasers in the $z$ direction and the ones in the $x - y$ plane, the angle $\beta \in \{0, \pi/2\}$ controls the barrier height of adjacent double-well minima, while

$$\theta \in \{-\pi, \pi\},$$

controls the energy offset (tilt) between these minima. In particular, as illustrated in Fig. 2, tuning the angle $\beta$ from 0 to $\pi/2$ results in a vanishing intermediate barrier between adjacent minima, thus resulting in a single central minimum.
Having presented the full optical potential of a DWOL, it is pertinent to find its approximate form $V(x, y, z)$ (with terms up to quadratic order) that is of interest for our further discussion. Given that the DWOL configuration can be tuned by varying $\beta$ and $\theta$ (for an illustration, see Fig. 3) we will approximate the full DWOL potential around the point $[-\lambda_L/4, 0, 0]^T$ in the $x - y$ plane. We do so assuming that $\xi_z \ll w_{0,x}/\xi_x, w_{0,y}/\xi_y$, which ensures that the cross term $\hat{U}_{\text{cr}}$ in Eq. (11) gives rise to only a small disturbance of the DWOL in the $x - y$ plane. In order to determine the approximated potential $V(x, y, z)$ we introduce the new variable $\hat{x} \equiv x + \pi/(2k_L)$. We also assume that $|\hat{x}|/Z_{R,x} \ll 1$, $|y|/Z_{R,y} \ll 1$, $|\hat{x}|/w_{0,x} \ll 1$, $|y|/w_{0,y} \ll 1$, $k_z |z| \ll 1$, $k_L |\hat{x}| \ll 1$, and $k_L |y| \ll 1$. Based on these assumptions, we straightforwardly obtain

$$V_D = -V_{d,0} + m a_x x + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) , \quad (12)$$

where

$$\frac{V_{d,0}}{U_{d,0}} = 4 \left[ \cos^2 \left( \frac{\beta}{2} \right) + 2 \cos^4 \left( \frac{\theta}{2} \right) \sin^2 \left( \frac{\beta}{2} \right) \right] . \quad (13)$$

The squared frequencies in Eq. (12) are given by

$$\omega_x^2 = \frac{4 U_{d,0} k_z^2}{m} \left\{ \cos \theta + \cos (2\theta) \right\} \sin^2 \left( \frac{\beta}{2} \right) + \cos^2 \left( \frac{\beta}{2} \right) ,$$

$$\omega_y^2 = \frac{4 U_{d,0} k_z^2}{m} \left[ 1 + \cos \theta \sin \left( \frac{\beta}{2} \right) \right] , \quad (14)$$

$$\omega_z^2 = \frac{2 U_{d,0} k_z^2}{m} \left\{ \xi_z + \sqrt{\xi_z} \left[ \cos \left( \frac{\phi}{2} \right) + \sin \left( \frac{\phi}{2} \right) \right] \right\} ,$$

while the expression for the factor $a_x$, which has dimensions of acceleration, reads

$$a_x = -\frac{4 U_{d,0} k_z^2}{m} \sin^2 \left( \frac{\beta}{2} \right) (1 + \cos \theta) \sin \theta . \quad (15)$$

It is pertinent at this point to underscore two important properties of the approximated potential $V_D$ of interest for our further discussion. Firstly, by contrast to the total DWOL potential that is nonseparable in the $x - y$ plane, this approximated potential is separable, which simplifies the treatment of atom transport governed by it. Secondly, in addition to quadratic terms, characteristic of linear harmonic oscillators, this potential also contains a term linear in $x$.

C. AOM configurations for atom transport

To set the stage for further discussion of atom transport in DWOIs, we first specify the relevant configurations of AOMs that enable transport along $x$, $y$, and diagonal ($r$) directions (for a schematic illustration, see Figs. 3 and 4).

To understand the proposed configurations, it is instructive to first recall how the use of an AOM engenders the basic moving-lattice effect. Generally speaking, AOMs can shift an incoming frequency by applying an ultrasonic frequency onto a crystal resulting in a density modulation along that crystal. Consequently, the incoming laser light encounters the density modulations that effectively play the role of a grating, thus leading to diffraction. Therefore, the application of the AOM leads to a frequency shift by the amount equal to the frequency of the ultrasonic sound wave $f_0$. The AOMs are connected to different channels of the direct-digital-synthesizer (DDS), which control the frequencies $f_1$ and $f_2$ applied to the crystals in the AOM. While one AOM ramps the frequency upwards, the other one turns it down by the same amount, thus leading to a detuning $\Delta f = f_1 - f_2 = c (|k_+| - |k_-|) / (2\pi)$ between the counterpropagating laser beams with wave-numbers $|k_+|$ and $|k_-|$, respectively. This results in an optical lattice moving with velocity $v = \pi \Delta f / k_L$, where $k_L = |k_L|$ is the laser wave number $\omega_0$.

Tuning one of the AOMs up in frequency and the other one down gives rise to a frequency difference between the beams with wave vectors $k_1$ and $k_3$. The same can be done with the pair of beams with wave vectors $k_2$ and $k_4$. Therefore, a moving-lattice effect in the corresponding directions is achieved. However, with the above realization one needs to tune both AOMs to achieve a displacement. Hence, the two pairs of laser beams will always undergo the same displacement in their respective directions. As a result, atom transport with this configuration of AOMs is only possible in the direction represented by the dashed line in Fig. 3 in the trivial case of equal frequencies in the
FIG. 4: (Color online) Schematic of a setup that enables a 2D lattice formed by four different beams. The two AOMs for one pair of counterpropagating beams tune the frequency up and down, respectively, resulting in a moving DWOL within the $x - y$ plane. They are controlled separately through the DDS system. An additional pair of counterpropagating laser beams, not shown here, forms an optical lattice in the $z$ direction.

To provide implementations for a broader set of displacement schemes and different values of the parameters $\beta$ and $\theta$, a more sophisticated experimental setup is required. As it turns out, to enable transport in an arbitrary direction within the $x - y$ plane one ought to forgo the retroreflected beams and the ensuing intrinsic phase stability, introducing instead two additional AOMs to the system. This approach, illustrated in Fig. 4, allows one to separately address the beams in the $x$- and $y$ directions by tuning the corresponding pairs of AOMs. In this manner, it is possible to have different lattice displacements in those two directions.

It should be stressed that, unlike DWOLs formed from a folded retroreflected beam, the chosen setup requires active phase stabilization to counteract the effects of mirror-induced phase noise. Namely, it is known that a $D$-dimensional optical lattice, created with no more than $D + 1$ independent light beams is topologically stable to arbitrary changes of the relative phases of the $D + 1$ beams. However, the DWOL in the $x - y$ plane ($D = 2$) is created by 4 beams, which is more than $D + 1 = 3$, hence active stabilization of the relative phase between standing waves is needed here.

III. STA-BASED TRAJECTORIES

Inverse engineering based on LRIs is the most widely used approach for modelling atomic transport. In particular, the basic LRI-based transport theory, developed in Ref. [5], makes use of a particular family of quadratic-in-momentum invariants [40]. One of the crucial implications of that theory is that the harmonic-trapping case and that of an arbitrary trap entail different treatments. Namely, the perfect transport in the latter case necessitates, in principle, the use of compensating forces in the comoving reference frame of the trap (cf. Sec. V C).

In the following, we apply the STA theory of Ref. [5] to determine the classical path of the potential minima in a moving DWOL. We do that using a single-atom Hamiltonian with the harmonically approximated DWOL potential of Eq. (12). To begin with, we briefly summarize the main concepts behind the inverse-engineering approach based on LRIs (for a more detailed introduction, see, e.g., Ref. [37]).

A. Inverse-engineering approach to atom transport

For a time-dependent Hamiltonian $H(t)$, any operator $I(t)$ that satisfies the equation

$$\frac{\partial}{\partial t} I(t) + [H(t), I(t)] = 0$$

(16)

constitutes a dynamical invariant of this Hamiltonian. One immediate consequence of the last equation is that the eigenvalues $\lambda_n$ of $I(t)$ are time-independent. If these eigenvalues are also non-degenerate, the corresponding eigenstates $|\Phi_n(t)\rangle$ and the instantaneous eigenstates $|\Psi_n(t)\rangle$ of the Hamiltonian $H(t)$, referred to as transport modes of $H(t)$, are connected through the relation $|\Psi_n(t)\rangle = e^{i\theta_n(t)}|\Phi_n(t)\rangle$; here $\theta_n(t) = \frac{\hbar}{\mu} \int_0^t \langle\Phi_n(t')|[i\hbar \partial_t V(t') - H(t')]|\Phi_n(t')\rangle dt'$ stands for the Lewis-Riesenfeld phase. As a result, the general solution of the Schrödinger equation for $H(t)$ can succinctly be written in the form

$$|\Psi(t)\rangle = \sum_n C_n e^{i\theta_n(t)}|\Phi_n(t)\rangle.$$  

(17)

An important class of Hamiltonians used in modelling atom transport are those of the Lewis-Leach type [66]. The latter are given by

$$H(t) = \frac{p^2}{2m} + V(q, t),$$

(18)

where the potential $V(q, t)$ in the most general case reads

$$V(q, t) = -F(t)q + \frac{m}{2} \omega^2(t)q^2 + \frac{1}{\rho^2(t)} \frac{q - \alpha(t)}{\rho(t)}.$$

(19)

with $\rho(t)$, $\alpha(t)$, $\omega(t)$, and $F(t)$ being arbitrary functions of time that satisfy the auxiliary equations [5]

$$\ddot{\rho} + \omega^2(t)\rho = \frac{\omega_0^2}{\rho^2},$$

(20)

$$\ddot{\alpha} + \omega^2(t)\alpha = \frac{F(t)}{m},$$

(21)

where $\omega_0$ is a constant. The quadratic-in-momentum invariant corresponding to the general Hamiltonian of
Eq. (18), up to a constant factor, is given by
\[
I(t) = \frac{1}{2m} \left[ \rho(p - m\dot{\alpha}) - m\dot{\rho}(q - \alpha) \right]^2 \tag{22}
\]
In line with the standard practice [3], we further add to \( V_D \) and \( V_D^* \) the irrelevant time-dependent global terms \( m\omega_x^2 q_{0,x}(t) \) and \( m\omega_y^2 q_{0,y}(t) \), respectively, which do not give rise to any force. As a result, the auxiliary equations of the forced-harmonic-oscillator type are here given by

\[
\dot{q}_{c,x}(t) + \omega_x^2 [q_{c,x}(t) - q_{0,x}(t)] = -a_x, \tag{27}
\]
\[
\dot{q}_{c,y}(t) + \omega_y^2 [q_{c,y}(t) - q_{0,y}(t)] = 0, \tag{28}
\]
where \( q_c(t) \equiv [q_{c,x}(t), q_{c,y}(t), 0]^T \) stands for the corresponding 2D classical-particle trajectory.

The most interesting aspect of the last auxiliary equations is the presence of \( a_x \) on the right-hand-side (RHS) of Eq. (27), which results from the existence of terms linear in \( x \) in the approximated potentials \( V_D \) [cf. Eq. (12)]. The presence of \( a_x \) makes the problem at hand analogous to transport problems that involve a constant force (e.g., gravity) [3]. It is straightforward to see that Eq. (27) can be reduced to the form of Eq. (28) by a slight redefinition of \( \dot{q}_{c,x}(t) \), i.e., by introducing \( \dot{q}_{c,x}(t) \equiv q_{c,x}(t) + a_x/\omega_x^2 \). In this way, we reduce the problem of atom transport in the \( x \) direction, equally like the one in the \( y \) direction, to a known class of atom-transport problems solvable via inverse engineering [3].

By imposing appropriate boundary conditions for \( q_{0,x}(t) \) and \( q_{0,y}(t) \) – along with the corresponding condi-

\[ F_x(t) = m \left[ \omega_x^2 q_{0,x}(t) - a_x \right]. \tag{25}
\]

\[ F_y(t) = m\omega_y^2 q_{0,y}(t). \tag{26}
\]
tions for $q_{c,x}(t)$ and $q_{c,y}(t)$ consistent with Eqs. [27] and [25] – the general solution for the path of the potential minimum can be sought in the form of the ninth-degree polynomial [33]

$$q_{0,u}(t) = d_u \sum_{n=0}^{9} b_{n,u} \left( \frac{t}{t_i} \right)^n \quad (u = x, y),$$  \hspace{1cm} (29)

where $d_u$ is the transport distance (cf. Sec. IIIA). By taking into account the relevant initial/boundary conditions [33], the following solution for constants $b_{n,u}$ is obtained:

$$b_{3,u} = 2520 (t_i \omega_u)^{-2}, \quad b_{4,u} = -12600 (t_i \omega_u)^{-2},$$
$$b_{5,u} = 22680 (t_i \omega_u)^{-2} + 126,$$
$$b_{6,u} = -17640 (t_i \omega_u)^{-2} - 420,$$
$$b_{7,u} = 5040 (t_i \omega_u)^{-2} + 540,$$
$$b_{8,u} = -315, \quad b_{9,u} = 70. \quad \hspace{1cm} (30)$$

The obtained solution for the STA-based trap trajectory, i.e. path of the potential minimum, is illustrated by Fig. 4 which shows its $x$ component $q_{0,x}$ as a function of the transport time $t_i$.

IV. eSTA-BASED TRAJECTORIES

Despite the fact that STA have proven their worth in a variety of quantum systems [37], their modification – known as eSTA – has recently been proposed [38]. The principal motivation behind this method, which is inspired by optimal-control techniques [67], is to enable the design of efficient control protocols for systems that are not directly amenable to an STA-type treatment. The main idea behind eSTA is to approximate the Hamiltonian of such a system by a simpler one for which an STA-based protocol can straightforwardly be found. Under the assumption that this STA-based protocol is nearly optimal even when applied to the original system Hamiltonian, its sought-after eSTA counterpart is obtained using a gradient expansion in the control-parameter space.

This last assumption underscores the heuristic character of eSTA, which – in principle – does not guarantee its superiority over STA [38]. However, it was already demonstrated that eSTA outperforms STA in certain classes of quantum-control problems [38].

Having found the STA solution for the simplified harmonic DWOL potential in Sec. IIIA in what follows we apply the eSTA scheme to the same problem. To start with, we briefly review the basic concepts and assumptions behind this method.

A. Basics of the eSTA method

The first step required for the application of the eSTA method to a system described by the Hamiltonian $H_S$ amounts to finding an STA solution, parameterized by a vector $\lambda_0 \in \mathbb{R}^n$, for a “close” Hamiltonian $H_0$ [38]. It is assumed that there exists a parameter $\mu$, such that a series expansion of the type

$$H_S = \sum_{k=0}^{\infty} \mu^k H^{(k)},$$  \hspace{1cm} (31)

involves $H_0$ as its zeroth-order term [i.e. $H^{(0)} \equiv H_0$]. In the system under consideration, the role of $H_S$ is played by $H_D(t)$ of Eq. [33]. At the same time, $H_0$ is represented by the Hamiltonian $H_{D,0}(t)$ of Eq. [23].

Aiming to find an optimal solution for $H_S$ based on a previously obtained STA solution for $H_0$, the general control vector $\lambda_S$ of the full system can be expressed as a sum of the STA control vector $\lambda_0$ and an auxiliary control vector $\alpha$, i.e. $\lambda_S = \lambda_0 + \alpha$. The special value of $\alpha$ that corresponds to the sought-after optimal solution, i.e. the optimal eSTA correction vector, will be denoted by $\epsilon$ in what follows.

The main assumption underlying the eSTA scheme is that the STA-based protocol corresponding to the simplified Hamiltonian $H_0$ is close to being optimal when applied to the full Hamiltonian $H_S$ [38]. Another crucial assumption of the eSTA approach is that the deviation of the fidelity $F$ around its maximal value depends quadratically on the difference $\alpha - \epsilon$. In other words, the fidelity satisfies the approximate relation [38]

$$F\left(\mu_S, \lambda_0 + \alpha, \frac{\nabla F(\mu_S, \lambda_0)}{||\nabla F(\mu_S, \lambda_0)||}\right) \approx 1 - c (\alpha - \epsilon)^2,$$  \hspace{1cm} (32)

where $\epsilon \equiv ||\epsilon||$, $\alpha \equiv ||\alpha||$, and $c$ is a positive constant. Beased on the above assumptions and a Taylor expansion of the left-hand-side of Eq. [32] around $\epsilon = \alpha$, one straightforwardly obtains [38]

$$\epsilon \approx 2 \frac{[1 - F(\mu_S, \lambda_S)]}{||\nabla F(\mu_S, \lambda_0)||^2} \frac{\nabla F(\mu_S, \lambda_0)}{||\nabla F(\mu_S, \lambda_0)||^2}.$$  \hspace{1cm} (33)

Up to second order in $\mu_S$ the fidelity is given by [38]

$$F(\mu_S, \lambda_S) \approx 1 - \frac{1}{\hbar^2} \sum_{n=1}^{\infty} |G_n|^2,$$  \hspace{1cm} (34)

where $G_n$ is an auxiliary scalar function, given in terms of the transport modes of $H_0$ [cf. Sec. III] by

$$G_n = \int_0^{t_i} dt \langle \Psi_n(t) | [H_S(\lambda_0 ; t) - H_0(\lambda_0 ; t)] | \Psi_0(t) \rangle.$$  \hspace{1cm} (35)

Similarly, up to second order in $\mu_S$ the gradient of $F(\mu_S, \lambda_0)$ is given by an analogous approximate expression: [38]

$$\nabla F(\mu_S, \lambda_0) \approx - \frac{2}{\hbar^2} \sum_{n=1}^{\infty} \text{Re} (G_n K_n^*).$$  \hspace{1cm} (36)
Here $K_n$ is an auxiliary vector function:

$$K_n = \int_0^{t_f} dt \langle \Psi_n(t) | \nabla \lambda H_S(\lambda; t) |_{\lambda = \lambda_0} | \Psi_0(t) \rangle. \quad \text{(37)}$$

The optimal eSTA correction vector $\epsilon$ can be expressed in terms of $G_n$ and $K_n$ as

$$\epsilon = -\frac{\sum_{n=1}^{N} (G_n)^2 \sum_{n=1}^{N} \text{Re} (G_n^* K_n)}{\left| \sum_{n=1}^{N} \text{Re} (G_n^* K_n) \right|^2}, \quad \text{(38)}$$

where $N$ is the cut-off parameter. Based on this expression, $\epsilon$ can straightforwardly be calculated numerically provided that $G_n$ and $K_n$ are previously obtained by evaluating the integrals in Eqs. (33) and (37), respectively. In the problem under consideration, where $|\Psi_n(t)\rangle$ are the transport modes of a time-dependent 3D harmonic-oscillator Hamiltonian, the evaluation of those integrals is highly nontrivial and entails the use of various properties of Hermite polynomials [68] (for detailed derivations, see Appendices A and B).

### B. eSTA moving-lattice trajectories

In the transport problem at hand, the $x$- and $y$ components of the trap-trajectory vector, $q_{0,x}(\lambda_x; t)$ and $q_{0,y}(\lambda_y; t)$, are parametrized by the twelve-component real-valued control vector $\lambda = (\lambda_x, \lambda_y)^T$. Here $\lambda_x = [\lambda_x^{(1)}, \ldots, \lambda_x^{(6)}]$ and $\lambda_y = [\lambda_y^{(1)}, \ldots, \lambda_y^{(6)}]$ are the reduced six-component control vectors corresponding to the displacements in the $x$- and $y$ directions, respectively, which are assumed to satisfy the following conditions:

$$q_{0,x}(\lambda_x; \lambda_f/7) = \lambda_x^{(j)} \quad (j = 1, \ldots, 6),$$

$$q_{0,y}(\lambda_y; \lambda_f/7) = \lambda_y^{(j)}. \quad \text{(39)}$$

The STA-based trajectory corresponds to the control vector $\lambda = (\lambda_x,0; \lambda_y,0)^T$, with components $\lambda_x^{(j)}$ and $\lambda_y^{(j)}$ ($j = 1, \ldots, 6$). Thus, this trajectory will be denoted by $q_{0,x}(\lambda_x,0; t)$ and $q_{0,y}(\lambda_y,0; t)$. At the same time, the sought-after optimized (eSTA) trajectory corresponds to the control vectors $\lambda_x$ and $\lambda_y$, hence it will be denoted by $q_{0,x}(\lambda_x; t)$ and $q_{0,y}(\lambda_y; t)$.

The optimized (eSTA) paths of the potential minimum can be expressed through their STA counterparts as

$$q_{0,x}(\lambda_x; t) = q_{0,x}(\lambda_x,0; t) + f_x(\alpha_x; t),$$

$$q_{0,y}(\lambda_y; t) = q_{0,y}(\lambda_y,0; t) + f_y(\alpha_y; t), \quad \text{(41)}$$

where $\alpha := (\alpha_x, \alpha_y)^T$ is an auxiliary twelve-component control vector. These eSTA paths are assumed to satisfy the conditions expressed by $q_{0,x}(\lambda_x; \lambda_f/7) = \lambda_x^{(j)} + \alpha_x^{(j)}$ and $q_{0,y}(\lambda_y; \lambda_f/7) = \lambda_y^{(j)} + \alpha_y^{(j)}$ ($j = 1, \ldots, 6$). The auxiliary functions $f_u(\alpha_u; t)$ ($u = x, y$) have to obey the following boundary conditions:

$$f_u(\alpha_u; 0) = f_u(\alpha_u; \lambda_f) = 0,$$

$$f_u(\alpha_u; \lambda_f/7) = \alpha_u^{(j)} \quad (j = 1, \ldots, 6),$$

$$\frac{d^n}{dt^n} f_u(\alpha_u; t')|_{t' = 0, \lambda_f} = 0 \quad (n = 1, \ldots, 4). \quad \text{(42)}$$

The latter conditions are chosen such that $f_u(\alpha_u; t)$ can be controlled through $\alpha_u$, obeying at the same time the continuity conditions. Thus, we choose the following polynomial Ansatz of eleventh degree:

$$f_u(\alpha_u; t) = \sum_{n=0}^{11} \sum_{j=1}^{6} \tilde{a}^{(j)}_{u,n} \alpha_u^{(j)} \left(\frac{t}{\lambda_f}\right)^n. \quad \text{(43)}$$

The values of the coefficients $\tilde{a}^{(j)}_{u,n}$ and $\tilde{a}^{(j)}_{u,n}$ in the last equations are given in Table I of Ref. [68].

The auxiliary control vector $\alpha$ that corresponds to the sought-after eSTA solution is given by the twelve-component optimal correction vector $\epsilon \equiv (\epsilon_x, \epsilon_y)^T$, where $\epsilon_x$ and $\epsilon_y$ are evaluated using the general expression in Eq. (38). Given that in our 3D problem the transport modes can be enumerated by three 1D quantum numbers $\{n_x, n_y, n_z\}$, we can recast the sum in Eq. (38) in terms of the main quantum number $n$ and $\{n_x, n_y, n_z\}$. For the cut-off parameter $N$ we take the value $N = 2$, despite the fact that our numerical evaluations show that it suffices to take $N = 1$.

The $x$ component of a typical eSTA-based trajectory is depicted in Fig. 8. By comparing this trajectory to the STA-based one (cf. Fig. 5) it can be inferred that their shapes differ significantly only for short transport times.

### V. SINGLE-ATOM DYNAMICS

Having described the design of STA-based trap trajectories in Sec. IV and their eSTA-based counterparts in Sec. V, in the following we briefly present our chosen approach for evaluating the resulting single-atom dynamics. We start by reviewing the basic aspects of the use of the Fourier split operator method (FSOM) for solving time-dependent Schrödinger equations (TDSEs) in Sec. VA and for computing ground-state properties in Sec. VB. We then discuss our approach for numerically solving the relevant comoving-frame TDSE (Sec. VC), followed by the relevant details of the numerical implementation (Sec. VD).

#### A. Basic aspects of the FSOM

The FSOM has established itself as the method of choice for solving Cauchy-type initial-value problems $\partial_t f(r,t) = \hat{A}(r,t) f(r,t)$, where $\hat{A}(r,t)$ is an operator, possibly time-dependent, and the initial condition reads $f(r,t) = f_0(r)$. This method is particularly convenient
function \( \Psi(r, t) \): 
\[
\Psi(r, t + \delta t) = \exp \left[ -\frac{i}{\hbar} U(r) \frac{\delta t}{2} \right] \exp \left( \frac{i \hbar \nabla^2}{2m} \delta t \right) \times \exp \left[ -\frac{i}{\hbar} U(r) \frac{\delta t}{2} \right] \Psi(r, t) + \mathcal{O}(\delta t^3). \tag{46}
\]

In particular, the last equation allows one to treat the different exponential terms independently. Thus, it is pertinent to Fourier-transform the kinetic term to momentum space, noticing at the same time that the RHS of Eq. \((46)\) can be recast using the identity
\[
\exp \left( \frac{i \hbar \nabla^2}{2m} \delta t \right) \exp \left[ -\frac{i}{\hbar} U(r) \frac{\delta t}{2} \right] \Psi(r, t) = F^{-1} \left[ e^{-i \frac{\hbar \mathbf{k}^2}{2m} \delta t} F \left\{ \exp \left[ -\frac{i}{\hbar} U(r) \frac{\delta t}{2} \right] \Psi(r, t) \right\} \right],
\]
where \( F[\ldots] \) denotes the Fourier transform of the argument and \( F^{-1}[\ldots] \) its inverse.

A numerical solution of a TDSE at time \( t' = t + N_s \delta t \) is obtained by applying \( N_s \) times in succession the time-propagation scheme based on Eq. \((46)\) on an initial wavefunction \( \Psi(r, t) \). In numerical implementations of the FSOM, this wavefunction is discretized on a rectangular spatial grid with \( N_s \) points and the exact, continuous Fourier transform is approximated by its discrete counterpart. The computational burden of propagating the function \( \Psi(r, t) \) is dominated by the needed spatial Fourier transformation and its inverse. When carried out using the fast Fourier transform (FFT) algorithm \([72]\), an elementary step in these transformations within the framework of the FSOM requires \( \mathcal{O}(N_s \log N_s) \) operations.

### B. Ground-state calculation: Imaginary-time evolution approach

Apart from our use of the FSOM for the treatment of single-atom dynamics, we also utilize this method within the framework of the imaginary-time evolution (ITE) approach to determine the ground state of our DWOL optical potential. In particular, the ground-state wave function found in this manner represents the initial \((t = 0)\) atomic wave packet—the initial condition for single-atom dynamics. In what follows, we briefly review the ITE approach, which represents one of the most robust computational approaches for obtaining the ground state of a quantum system \([68, 74]\). We do so using the abstract, representation-independent notation.

Assuming that \( H \) is the Hamiltonian whose ground state one aims to determine, one expands the quantum state \( |\phi\rangle \) in terms of the eigenstates \( \{|\psi_n\rangle, n = 0, 1, \ldots\}\) of \( H \), i.e. \( |\phi\rangle = \sum_n c_n |\psi_n\rangle \). It is assumed that the sought-after ground state \( |\psi_0\rangle \) has a nonvanishing contribution to this expansion, i.e. \( c_0 \equiv \langle \psi_0 |\phi\rangle \neq 0 \). Assuming that
the system is initially \((t = 0)\) in the state \(|\phi\rangle\), its states at later times \(t\) are given by
\[
|\phi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |\psi_n\rangle ,
\]
with \(E_n\) being the eigenvalue of \(H\) corresponding to the eigenstate \(|\psi_n\rangle\).

By switching from real to imaginary time \(t \rightarrow \tau = it\), i.e. performing a Wick rotation into the complex plane, Eq. (48) adopts the form
\[
|\phi(\tau)\rangle = \sum_n c_n e^{-E_n \tau/\hbar} |\psi_n\rangle .
\]
The last equation expresses \(|\phi(\tau)\rangle\) as an exponentially-decaying superposition of the eigenstates \(|\psi_n\rangle\) with the decay rates given by the corresponding eigenvalues \(E_n\). Because the exponential-decay rate of the ground state is the smallest one, in the large-\(\tau\) limit one obtains
\[
|\phi(\tau)\rangle \approx c_0 e^{-E_0 \tau/\hbar} |\psi_0\rangle .
\]
This implies that, given a trial state \(|\phi(\tau = 0)\rangle \equiv |\phi\rangle\) with a nonzero overlap with the actual ground state, the ITE approach engenders a monotonously decreasing functional of \(\tau\) that converges to the ground-state energy as \(\tau \rightarrow \infty\). In other words, \(E_0 = \lim_{\tau \rightarrow \infty} \langle \phi(\tau) | H | \phi(\tau) \rangle\).

In the problem at hand, we make use of the coordinate representation, thus the counterpart of Eq. (50) of interest for the present work then reads
\[
\phi(r, \tau) = \sum_n c_n e^{-E_n \tau/\hbar} \psi_n(r) ,
\]
where \(\phi(r, \tau) \equiv \langle r | \phi(\tau) \rangle\) and \(\psi_n(r) \equiv \langle r | \psi_n \rangle\) are the relevant wave functions.

For completeness, it is worthwhile to mention that the ground state of the DWOL potential can also be obtained to requisite accuracy using the plane-wave-expansion method (see, e.g., Ref. [15]). This approach is based on expanding the underlying periodic potential and the periodic part of single-particle Bloch wave functions in terms of reciprocal-lattice vectors.

The squared modulus \(|\psi_0(x, y, z = 0)|^2\) of the ground-state wave function, i.e. the ground-state probability density, in the \(x-y\) plane – computed using the ITE approach – is shown for one specific choice of system parameters in Fig. 7. The obtained bimodal shape of this probability density originates from the characteristic form of the ground-state wave function in a double well.

C. Relevant TDSE in the comoving frame and its FSOM-based numerical solution

The character of the problem at hand makes it prudent to switch from the lab frame to the one that corresponds to the DWOL (comoving frame). This change is effected through a generalized Galilean transformation [75]. The latter is represented by the unitary operator (see, e.g. Ref. [76])
\[
\hat{U} = e^{i \mathbf{p}_0 \mathbf{q}_0(t)/\hbar} e^{-i m \mathbf{r} \cdot \mathbf{q}_0(t)/\hbar} ,
\]
which transforms the relevant lab-frame TDSE
\[
i \hbar \frac{\partial}{\partial t} \Psi(r, t) = \left[ \frac{\mathbf{p}^2}{2m} + U_D(r - \mathbf{q}_0(t)) \right] \Psi(r, t)
\]
with the single-atom wave-function \(\Psi(r, t)\) into its counterpart in the comoving frame with its corresponding wave-function \(\Phi(r, t) \equiv \hat{U} \Psi(r, t)\):
\[
i \hbar \frac{\partial}{\partial t} \Phi(r, t) = \left[ \frac{\mathbf{p}^2}{2m} + m \mathbf{q}_0(t) \cdot \mathbf{q}_0(t)
\right.
- \left. m \mathbf{r} \cdot \mathbf{q}_0(t) + U_D(r) \right] \Phi(r, t) .
\]
It is important to stress that the terms \(m \mathbf{q}_0(t) \cdot \mathbf{q}_0(t)\) and \(m \mathbf{q}_0(t) \cdot \mathbf{q}_0(t)\) in Eq. (54) lead only to time-dependent global phase factors, which are immaterial for the atom-transport problem at hand. Therefore, these terms can henceforth be safely neglected and the total potential experienced by a transported atom in the comoving frame is given by \(W(r, t) \equiv U_D(r) + m \mathbf{r} \cdot \mathbf{q}_0(t)\).

In the atom-transport problem at hand, we make use of the FSOM to compute the final atomic state after center-of-mass displacement of the atomic wave packet by a certain distance. Because the potential \(W(r, t)\) carries an explicit time dependence, the exact time-evolution operator of the system is given by the most general expression that involves a time-ordered product. Yet, by making use of the identity in Eq. (15) for \(A = U_D(r)\) and \(B = \mathbf{p}^2/(2m) + m \mathbf{r} \cdot \mathbf{q}_0(t)\) the counterpart of the

FIG. 7: (Color online) The squared modulus \(|\psi_0(x, y, z = 0)|^2\) of the ground-state wave function (i.e. the ground-state probability density) in the \(x-y\) plane for \(U_{d,0} = 300 E_r\). The transverse beam waists are set to \(w_{x,y}/\lambda_L = 4.2 \times 10^3 \) cm. At the same time, the relevant angles are chosen such that \(\beta = 3\pi/20\) and \(\theta = \phi = \pi/2\).
time-stepping scheme of Eq. (46) in the atom-transport problem under consideration reads

\[ \Psi(r, t + \delta t) = \exp \left[ -\frac{i}{\hbar} U_D(r) \frac{\delta t}{2} \right] T_{r,p}(\delta t) \times \exp \left[ -\frac{i}{\hbar} U_D(r) \frac{\delta t}{2} \right] \Psi(r, t) + O(\delta t^3), \quad (55) \]

where \( T_{r,p}(\delta t) \) is defined as

\[ T_{r,p}(\delta t) = \exp \left[ -\frac{i}{\hbar} \left( \frac{\mathbf{p}^2}{2m} \delta t + m\mathbf{\ddot{r}} \cdot \int_t^{t+\delta t} \mathbf{\dot{q}}_0(t') dt' \right) \right]. \quad (56) \]

Using the Baker-Campbell-Hausdorff formula [71] and its immediate implications, we can recast \( T_{r,p}(\delta t) \) as (for a detailed derivation, see Appendix C)

\[ T_{r,p}(\delta t) = \exp \left[ -\frac{i}{\hbar} \frac{\mathbf{p}^2}{2m} \delta t \right] \exp \left[ -\frac{i}{2\hbar} \mathbf{\dot{p}} \cdot \delta \mathbf{q}_0(t) \delta t \right] \times \exp \left[ -\frac{i}{\hbar} m\mathbf{\ddot{r}} \cdot \delta \mathbf{q}_0(t) \right], \quad (57) \]

where \( \delta \mathbf{q}_0(t) \equiv \mathbf{q}_0(t + \delta t) - \mathbf{q}_0(t) \). It is worthwhile mentioning that another two multiplicative terms – which do not depend on the momentum- and coordinate operators and lead to irrelevant time-dependent global phase factors – have been omitted on the RHS of the last equation, by analogy to the omitted terms of Eq. (54) above.

By making use of an analog of Eq. (47) and performing a Fourier transformation of the \( \mathbf{p} \)-dependent terms in (57) [switching also to the coordinate representation of the momentum operator \( \mathbf{p} \rightarrow (\hbar/i)\nabla \)], we finally find that the FSOM-based second-order time-stepping scheme for the atom-transport problem at hand is given by:

\[ \Phi(r, t + \delta t) = \exp \left[ -\frac{i}{\hbar} U_D(r) \frac{\delta t}{2} \right] \mathcal{F}^{-1} \left[ e^{-\frac{i\mathbf{k} \cdot \delta \mathbf{q}_0}{\hbar}} \right] \times \exp \left[ -\frac{i}{\hbar} \mathbf{k} \cdot \delta \mathbf{q}_0 \delta t \right] \mathcal{F} \left\{ \exp \left[ -\frac{i}{\hbar} m\mathbf{\ddot{r}} \cdot \delta \mathbf{q}_0 \right] \right\} \times \exp \left[ -\frac{i}{\hbar} U_D(r) \frac{\delta t}{2} \right] \Phi(r, t) + O(\delta t^3). \quad (58) \]

The typical dynamics of an atomic wave-packet moving in the \( x \)-direction in a DWOL, evaluated by numerically solving the above TDSE in the comoving frame based on Eq. (58) with an eSTA-based moving-DWOL trajectory, are illustrated in Fig. 8. The three snapshots of the motion shown in this plot illustrate the characteristic incipient acceleration and the terminal slowing down in atomic transport. Namely, as can be inferred from Fig. 8, the distance covered in the first fifth of the total transport time \( t = t_f \) constitutes nearly one third of the total distance \( d_x \), while the one corresponding to the final fifth amounts to only 0.02 \( d_x \).

D. Details of the numerical implementation

For the sake of alleviating the computational burden in the problem under consideration, it is pertinent to make use of the discrete translational symmetry of the system and restrict ourselves to the displacement of one unit cell of the original DWOL. Needless to say, the appropriate choice of the unit cell has to be consistent with the transport direction. For instance, in order to evaluate transport in the \( x \)- and \( y \) directions we make use of a rectangular unit cell (indicated by white dashed lines in Fig. 1). At the same time, describing transport in the diagonal direction necessitates the use of a 45-degree rotated square-shaped unit cell (black dashed lines in Fig. 1).

Another problem-specific circumstance that allows one to further reduce the computational burden in the problem at hand is intimately related to its description in the comoving frame [cf. Sec. VI]. Namely, from the form of the relevant TDSE [cf. Eq. (54)] it can straightforwardly...
be inferred that there is no need to calculate the potential term after each time step. Instead, we need only evaluate the correction term \( m \mathbf{r} \cdot \mathbf{q}_0 \) [cf. Eq. (54)] that depends on the acceleration \( \mathbf{q}_0 \) of the potential minimum.

To carry out the spatial Fourier transformation, here implemented using the FFT algorithm [recall the discussion in Sec. (V A)], we make use of a discrete three-dimensional \( N_x \times N_y \times N_z \) grid with \( N_x = 200, N_y = 300, N_z = 100 \) points in the computational window whose respective dimensions (in units of \( l_x, l_y, l_z \)) are 100, 100, and 500. As for the numerical time-domain propagation of the relevant TDSE in the comoving frame [cf. Eq. (54)], we utilize the adaptive approach [73] with a maximal relative error of \( 10^{-4} \), which could – in principle – require additional (smaller) substeps in time. However, in all our runs, it was sufficient to take \( N_t \) between 20 and 100.

VI. TRANSPORT FIDELITY: RESULTS AND DISCUSSION

In the following, we discuss the efficiency of single-atom transport in a DWOL resulting from the STA- and eSTA-based trap trajectories [cf. Secs. III B and IV B, respectively]. The central figure of merit that quantifies the efficiency of atom transport is the transport fidelity \( \mathcal{F}(t_f) = |\langle \Psi_{\text{target}} | \Psi(t_f) \rangle|^2 \). The dependence of \( \mathcal{F} \) on the transport time \( t_f \) is determined by the overlap of the target state \( |\Psi_{\text{target}}\rangle \) (the ground state of the displaced DWOL potential) and the final atomic state \( |\Psi(t_f)\rangle \), obtained using the FSOM.

The obtained results for the transport fidelity in the DWOL system under consideration are illustrated in Figs. 9–12. One common feature of all these results, regardless of the concrete values of the system parameters (lattice depth, transport distance, beam waists, etc.), is the breakdown of transport – manifested by a sharp decrease in the fidelity – for short transport times \( t_f \). This characteristic breakdown results from the fact that for atomic accelerations above a certain maximal value \( |\dot{a}_{\text{max}}| \), which is proportional to the lattice depth [42], the transported atom cannot be confined by the optical-lattice potential. This coincides with the disappearance of the minima of the potential experienced by the atom in its comoving (non-inertial) reference frame, which differs from the potential in the lab frame by a term linear in the transport coordinate \( z \) (thus, effectively representing a tilted lattice potential). This behavior for short transport times is a generic characteristic of coherent atom transport in optical-lattice potentials, i.e. it is not specific only for DWOLs.

The aforementioned collapse actually takes place when the maximal atomic acceleration reached during the transport process, which will be denoted by \( |\ddot{a}_{\text{max}}| \) in what follows, exceeds \( |\dot{a}_{\text{max}}| \). The value of \( |\dot{a}_{\text{max}}| \) depends on the concrete moving-lattice trajectory (i.e. the path of the potential minimum), but it generally holds that \( |\ddot{a}_{\text{max}}| \propto t_f^{-2} \). This implies that for larger lattice depths (i.e. for higher |\dot{a}_{\text{max}}| \propto U_0) the largest atomic acceleration |\ddot{a}_{\text{max}}| reached exceeds |\dot{a}_{\text{max}}| at shorter transport times \( t_f \). Rephrasing, for deeper lattices (i.e. stronger lattice potentials) the collapse of the fidelity takes place for shorter times \( t_f \). Our numerical findings are in agreement with this general argument, as can be inferred from Figs. 9–12 for gradually increasing potential depths. The characteristic transport times \( t_f \) that correspond to the onset of the aforementioned breakdown are around \( 3.8 T_x \) and \( 3.3 T_x \), respectively, in Figs. 9 and 10. Therefore, they clearly show the anticipated trend of decreasing with the increase of the lattice depth. By contrast to this short-time behavior, in the opposite limit of very long transport times \( t_f \) both STA and eSTA results correspond to the well-known adiabatic limit. In other words, both methods allow one to achieve essentially perfect atom transport (\( \mathcal{F} \approx 1 \)) for \( t_f \gg \omega_n^{-1} (u = x, y) \).

By comparing the two methods used, the superiority

![Graph](attachment:image.png)
of the eSTA method over its STA counterpart for most transport times is easily noticeable. This superiority becomes more prominent for deeper lattices, which can be explained by the fact that the parameter $\mu_s$ [cf. Eq. (31)] depends on the characteristic wave number $k_L$ of the potential, while $k_L$ in turn depends on the lattice depth $U_{d,0}$ [i.e. $\mu_s \propto U_{d,0}^{-1/2}$]. Thus, larger lattice depths result in smaller values of $\mu_s$ and, consequently, in a better approximation of the optimization vector pertaining to the eSTA method [cf. Sec. IV A]. Furthermore, with increasing lattice depth the stability of the eSTA scheme is improving. This can readily be seen by the decrease of the oscillatory feature around $4.15 T_x$, $3.8 T_x$ in Figs. 10 and 11 respectively. However, this only holds true if eSTA already results in a significant improvement over STA, otherwise an increase of the lattice depth $U_{d,0}$ would lead to a more prominent oscillatory feature around $4.15 T_x$ and $3.7 T_x$ in Figs. 9 and 12 respectively.

To arrive at a more complete physical understanding of coherent atom transport in DWOLs, it is pertinent to also comment on the results for the transport fidelity [cf. Figs. 9 – 11] from the standpoint of of the characteristic shapes of the corresponding trajectories of a moving DWOL, as obtained using the STA- [cf. Fig. 5] and eSTA methods [cf. Fig. 6]. What can be inferred by inspecting those results is that the typical transport times $t_f$ required for a high-fidelity atom transport correspond to moving-DWOL trajectories that do not display oscillatory features. For example, the eSTA-based trajectory that corresponds to $t_f/T_x = 2$ in Fig. 6(a) clearly shows oscillating character, but does not permit high-fidelity atom transport in the $x$ direction. Similar conclusions can be drawn in connection with atom transport in other directions, discussed in what follows. Thus, in the DWOL system considered here only non-oscillatory solutions for the moving-DWOL trajectory can enable
high-fidelity transport.

Aside from the nonseparability of its underlying optical potential $U_D(x, y, z)$ in the $x-y$ plane [cf. Eq. (10)], one of the central features of the DWOL is the anisotropy of this potential. The results for atom transport in the $x-y$ plane are therefore strongly direction-dependent and exhibit different general behaviour, as can be inferred by comparing Figs. 10 and 11. Only the trivial parameter choices of $\beta = 0$ or $\beta = \pi/2$, with $\theta = \pi/2$, would result in a simpler form of the potential, which in those cases is similar to that of the ordinary (single-well) optical lattice $E_R$. 

Apart from the already discussed consequences of the anisotropic character of the underlying optical potential for atom transport, another effect specific for DWOLs is worthwhile being considered here. Namely, the presence of the intermediate potential barrier between the two wells within a double well has profound consequences for atom transport. By analogy to the existence of the maximal acceleration $|a_{\text{max}}|$ that a lattice can endure before atom transport breaks down (closely related, as explained above, to the dissappearance of minima of the potential in the reference frame moving with the transported atom), above a certain acceleration $|a_{\text{int}}|$—which is generally smaller than $|a_{\text{max}}|$—the intermediate barrier will cease to be a local maximum of the tilted lattice potential. Its transport implications are intimately related to the fact that once $|a_{\text{int}}|$ is exceeded the wave function of the transported atom becomes a mixture of the wave functions corresponding to adjacent single-well minima within the unit cell of a DWOL. Consequently, this leads to a noticeable drop in the transport fidelity.

The consequences of the existence of the intermediate potential barrier can be understood by comparing the fidelities shortly before the breakdown for transport in $x$- and $y$ directions [c.f. Figs. 10 and 11]. It is noticeable that the peak present around $3 T_y$ in Fig. 11 does not exist for its $x$-direction counterpart in Fig. 10. Only in the trivial cases $\beta = 0$ and $\beta = \pi/2$ the acceleration $|a_{\text{max}}|$ remains relevant, because in those cases all barriers between adjacent minima have the same height. In all other cases it is possible to exceed $|a_{\text{int}}|$ without exceeding $|a_{\text{max}}|$ for short enough transport times. Therefore, through the angle $\beta$ one can control the mixing of the wave functions corresponding to adjacent minima by controlling the height of the intermediate barrier. Accordingly, by tuning $\beta$ one can control the behaviour of the fidelity pertaining to the transport in the $x$ direction for times close to the breakdown time.

The diagonal displacement results in worse results for eSTA in comparison to STA, Fig. 12. However, this is not expected to be a direct problem with the 2D adaptation of the eSTA procedure but rather shows that the parameter pair of the distance and lattice depth is not suited for the displacement problem. Comparing parts (a) and (b) of Fig. 12 with (c) shows that an increase of the lattice depth results in a better performance of the eSTA method. Increasing the potential depth even further would result in a superior performance of eSTA over STA.

Having discussed both general atom-transport effects and those specific for DWOLs, for the sake of completeness it is pertinent to discuss the STA- and eSTA-based transport for very deep lattices ($U_{d,0} \gtrsim 1000 E_R$). It should be stressed, that the maximal lattice depth is in principle in multiple thousands of the recoil energy $E_R$ and is essentially determined by the available laser power, as well as the capability to sufficiently tightly focus the laser beam. In particular, Figs. 13–15 show different examples of transport in the $x$, $y$, and diagonal directions for different total transport distances, all of them obtained for $U_{d,0} = 1500 E_R$. 

The $x$-direction transport in the deep-lattice regime, illustrated by Fig. 13 shows a significantly better performance of eSTA in comparison to STA. In particular, in the close vicinity of the total breakdown around

![FIG. 12: (Color online) The dependence of the atom-transport fidelity on the transport time $t_t$, for a potential strengths $U_{d,0}$ (a) of $300 E_R$, (b) $400 E_R$ and (c) $600 E_R$. The transport distance $d_t$ along the diagonal was set to $448 l_x$. For the Gaussian beam along the $z$-axis the transverse beam waists were set to $w_{x/y,0} = 4.2 \times 10^3 l_x$. The relevant angles are chosen such that $\beta = 3\pi/20$ and $\theta = \phi = \pi/2$.](image-url)
FIG. 13: (Color online) The dependence of the atom-transport fidelity on the transport time \( t_f \), for a lattice depth \( U_{d,0} \) of 1500 \( E_R \). The transport distance \( d_x \) along the \( x \)-axis was set (a) to 127 \( l_x \), (b) 158 \( l_x \) and (c) 191 \( l_x \). For the Gaussian beam along the \( z \)-axis the transverse beam waists were set to \( w_{x/y,0} = 4.2 \times 10^3 \) \( l_x \). The relevant angles are chosen such that \( \beta = 3\pi/20 \) and \( \theta = \phi = \pi/2 \).

\( t_f \approx 2.75 \) \( T_x \) and \( t_f \approx 3.25 \) \( T_x \), the eSTA-based trajectories still allow one to reach fidelities above 0.9. By contrast to that, the fidelity of the STA-based transport falls below 0.9 for a transport distances of \( d_x = 158 \) \( l_x \) [see Fig. 13(b)], and even below 0.75 for distances of \( d_x = 191 \) \( l_x \) [cf. Fig. 13(c)].

The \( y \)-direction transport in the deep-lattice regime displays similar behavior to that of a simple optical conveyor belt \( \text{[33]} \), in that the local maxima reach nearly perfect fidelity before the occurrence of the transport breakdown. This is not completely surprising, however, because the two systems share a similar periodicity along the \( y \) direction. Furthermore, our results strongly suggest that even for very large lattice depths the eSTA procedure becomes more unstable for longer total transport distances. This trend is manifested by the growing oscillations in Fig. 14 resulting in a worse performance of eSTA than STA for final times around \( t_f \approx 3.7 \) \( T_y \). These oscillation are also clearly visible in Fig. 13(c) around \( t_f \approx 4.15 \) \( T_x \).

The results obtained for diagonal atom transport are even better for eSTA in comparison to STA and previously discussed parameter sets, this being manifested by (significantly) better or equal fidelity values for all probed final times above the breakdown time \( t_f \approx 3 \) \( T_x \). Even the oscillatory behaviour, which can be noticed in Fig. 13 (b) and (c) around \( t_f \approx 3.9 \) \( T_x \), results in higher fidelity values for eSTA in comparison to STA.

For the sake of completeness, it is worthwhile pointing out that – in addition to outperforming STA-based schemes in terms of achievable transport fidelity – the eSTA method also shows increased stability (i.e. robustness against errors) compared to its STA counterpart. That has quite recently been demonstrated on the example of atomic transport in conventional 1D optical lattices.

FIG. 14: (Color online) The dependence of the atom-transport fidelity on the transport time \( t_f \), for a potential strengths \( U_{d,0} \) of 1500 \( E_R \). The transport distance \( d_y \) along the \( y \)-axis was set (a) to 127 \( l_y \), (b) 158 \( l_y \) and (c) 191 \( l_y \). For the Gaussian beam along the \( z \)-axis the transverse beam waists were set to \( w_{x/y,0} = 4.2 \times 10^3 \) \( l_x \). The relevant angles are chosen such that \( \beta = 3\pi/20 \) and \( \theta = \phi = \pi/2 \).
The dependence of the atom-transport fidelity on the transport time $t_f$, for a lattice depth $U_d$ of $1500 E_R$. The transport distance $d_r$ along the diagonal was set to (a) $127 l_r$, (b) $158 l_r$, and (c) $191 l_r$. For the Gaussian beam along the $z$-axis the transverse beam waists were set to $w_{x,y} = 4.2 \times 10^3 l_x$. The relevant angles are chosen such that $\beta = 3\pi/20$ and $\theta = \phi = \pi/2$.

In that recent paper, a general heuristic argument that leads to this last conclusion was complemented by an extensive numerical investigation of the robustness of STA and eSTA schemes with respect to classical Gaussian white noise in the lattice depth and atomic position, as well as systematic errors in various system parameters (lattice depth, laser wave number, etc.).

While our principal goal in the present work was to devise control protocols that lend themselves to straightforward experimental implementations of fast atom transport, it is worthwhile to note that the obtained eSTA-based control protocols can serve as a convenient starting point for further numerical optimization. In this context, it is worth mentioning that the optimal-control approach to atom transport has recently been demonstrated on the example of a 1D optical lattice and proved capable of reaching the corresponding quantum speed limit [12].

A. Coherent atom transport in DWOLs as a prerequisite for neutral-atom QC

While long-range dipole-dipole interactions between Rydberg atoms are currently the most widely used physical mechanism for realizing entangling two-qubit gates for neutral-atom-based QC [22, 24], short-range (contact) interactions between atoms in their electronic ground states represent the main ingredient of an alternative approach [17, 20]. In this approach, a pair of atomic states (e.g., one from each hyperfine-split ground-state manifold of $^{87}$Rb) play the role of two logical qubit states $|0\rangle$ and $|1\rangle$. A pair of atoms acquires a time-dependent phase obtained using optimal-control methods – the transport times we found in the present work compare well with those of Ref. [12], even though they correspond to a different optical-lattice potential and transport distances. To be more specific, the transport distance in Ref. [12] was fixed to be 15 times larger than the linear dimensions of the atomic wave packet, while lattice depths up to $300 E_R$ were considered. The resulting shortest transport times were found to be roughly equal to the oscillation period corresponding to the harmonically approximated lattice potential. On the other, the transport distances discussed in the present work were at least an order of magnitude larger than those in Ref. [12] (i.e. more than 150 times larger than the size of the atomic wave packet) and we considered lattice depths up to $1500 E_R$. It is interesting to note that the transport times in Fig. 10, which we obtained in the similar range of lattice depths as in Ref. [12] and for a roughly ten times larger distance ($d_x = 158 l_x$), are between 3.5 and $4 T_x$. Another argument in favor of the conclusion that transport times found using the eSTA method are close to the quantum speed limit has quite recently been provided for a moving 1D optical lattice [39].

VII. QUANTUM-TECHNOLOGY IMPLICATIONS

Coherent atom transport in moving optical lattices and tweezers, typically modelled using the STA family of quantum-control methods (including the eSTA method), is a prerequisite for a number of applications in the realm of emerging quantum technologies. In what follows, we dedicate special attention to the implications of fast (nonadiabatic) atom transport in DWOLs for two of those application areas. Namely, we first discuss the role of such transport in neutral-atom QC, more precisely the realization of entangling two-qubit gates based on collisional interactions (Sec. VII A). We then discuss the implications of spin-dependent atom transport in DWOLs in quantum sensing – more specifically yet, measurements of homogeneous constant forces using guided-atom interferometry (Sec. VII B).
according to $|jj\rangle \rightarrow e^{iU_{jj'}t/\hbar}|jj\rangle$ ($j, j' = 0, 1$), where this phase is determined by the interaction strength $U_{jj'}$. The short-range nature of the atom-atom coupling ensures that only the desired pair of qubits participates in the entangling operation, thus eliminating the unwanted coupling to other qubits and the environment.

The principal idea behind the collisional-gate approach to neutral-atom QC is to merge two atoms, which were initially spatially separated, into a common optical trap such that their wave functions have significant overlap. This gives rise to a controlled atomic collision, which is either based on spin-dependent interaction, spin-dependent transport, or spin-exchange interactions. Following a time interval of fixed duration, which is set by the contact-interaction strength in the merged state, the two atoms can again be spatially separated. This is the characteristic three-stage merge-wait-separate sequence that underlies the realization of collisional two-qubit gates.

One typical two-qubit gate enabled by collisional spin-exchange interactions is the square-root-of-SWAP ($\sqrt{\text{SWAP}}$) [19], an entangling counterpart of the SWAP operation that exchanges the states of two qubits. For qubits indexed by $n$ and $n + 1$, this gate is given by

$$\sqrt{\text{SWAP}} = e^{i\frac{\pi}{8}e^{-i\frac{\pi}{8}(X_n \otimes X_{n+1} + Y_n \otimes Y_{n+1} + Z_n \otimes Z_{n+1})}}, \quad (59)$$

where $X_n, Y_n, Z_n$ are the Pauli operators of different qubits. Regardless of the specific QC platform used, $\sqrt{\text{SWAP}}$ represents the natural two-qubit gate in the presence of Heisenberg-type exchange interactions between adjacent qubits [77, 78]; together with single-qubit rotations it forms a universal gate set for QC [80]. Owing to their specific geometry and the dynamic-control capability (e.g. coherent splitting of atoms from single wells into double wells) [10], DWOLs were utilized for the experimental realization of the $\sqrt{\text{SWAP}}$ gate [51] based on the mechanism proposed in Ref. [81].

One of the crucial prerequisites for the collisional-interaction approach to realizing two-qubit gates – such as $\sqrt{\text{SWAP}}$ – with neutral atoms is to time-efficiently bring two atoms to the desired optical-lattice sites; in the context of DWOLs, this amounts to bringing atoms to adjacent single wells within a double well. Thus, high-fidelity nonadiabatic single-atom transport is of pivotal importance for the practical viability of this approach [19]. Moreover, because collisional gates are sensitive to the vibrational state, it is essential to avoid vibrational excitation at the end of transport. This last requirement speaks in favor of using schemes based on STA in modelling such fast coherent transport (recall the discussion in Sec. 1). The eSTA method, which provides a consistent improvement compared to STA in terms of achievable transport fidelities (as discussed in Sec. VI), being at the same time more robust to decoherence and noise [59], appears as the likely method of choice for designing the desired transport trajectories.

B. Spin-dependent atom transport in DWOLs for quantum sensing via guided-atom interferometry

In recent years atom interferometry [52] has facilitated significant progress towards quantum-enhanced sensors. The principal idea underlying the operation of an atom interferometer is to first split and then – after some time – recombine atomic wave function. By detecting the differential phase accumulated during the separation period, one can extract small potential differences between the arms of an interferometer. While still being less developed than its counterpart with freely falling atoms, interferometry based on trapped atoms is advancing rapidly.

One specific direction within this field that has attracted considerable attention in recent years is STA-mediated guided interferometry that allows measurements of homogeneous constant forces [14, 12]. In compact atom interferometers envisioned to be used for this purpose the atom is driven by spin-dependent trapping potentials that are assumed to move in opposite directions; these spin-dependent potentials are complemented by linear and time-dependent potentials that can compensate the acceleration of the trap. While the pioneering work in this direction proposed the use of harmonic trapping potentials [15], it was subsequently understood that one can benefit from the use of moving optical lattices (i.e. anharmonic potential) [16], as the latter allow the atomic wave function to be localized with nanoscale spatial resolution. [Needless to say, the eSTA method can be used as an alternative to STA in designing moving-lattice trajectories.] As a result, precise measurements at ultrashort spatial scales can be performed.

In order to create two spin-dependent moving optical lattices, one makes use of a specially chosen wavelength of light that allows atoms in the state $|\uparrow\rangle$ to be trapped only by the right-handed circularly polarized light, while atoms in the state $|\downarrow\rangle$ are predominantly trapped by the left-handed circularly polarized light [12]. To be more specific, to coherently transport atoms in this way (selectively in either one of the two relevant spin states) one makes use of a polarization-synthesized beam, where the phases and amplitudes of its left- and right-handed circularly polarized components are steered with high precision. When the polarization-synthesized beam interferes with a counterpropagating reference beam of fixed linear polarization, two superposed standing waves are created.

The envisioned Ramsey-type interferometer makes use of atoms that have two internal states – the spin-up state $|\uparrow\rangle$ and the spin-down state $|\downarrow\rangle$. The state of the atom at time $t$ is given by $\xi_{\uparrow} |\uparrow\rangle \psi_{\uparrow\downarrow}(x, t) + \xi_{\downarrow} |\downarrow\rangle \psi_{\downarrow\downarrow}(x, t)$, where $\psi_{\uparrow\downarrow}(x, t) \equiv \langle x|\psi_{\uparrow\downarrow}(t)\rangle$ are the coordinate parts of the total atom wave functions in the two internal states. Assuming that one starts with the initial spin-up state of the system, a $\pi/2$ pulse gives rise to a coherent superposition of spin-up and spin-down states with equal weights (i.e. $\xi_{\uparrow} = \xi_{\downarrow} = 1/\sqrt{2}$). Then the two internal states are spatially separated and recombined. As a consequence of the presence of spin-dependent potentials, the
two spin components evolve differently. At the final time \( t = t_f \), where \( t = 0 \) corresponds to the end of the \( \pi/2 \) pulse, the differential phase \( \Delta \phi(t_f) \) is given by the complex argument of the relevant overlap \( \langle \psi^\uparrow(t_f) | \psi \uparrow(t_f) \rangle \), i.e. \( \langle \psi^\uparrow(t_f) | \psi \uparrow(t_f) \rangle = e^{i \Delta \phi(t_f)} \langle \psi^\uparrow(t_f) | \psi \uparrow(t_f) \rangle \). A second \( \pi/2 \) pulse allows one to extract the populations

\[
P_{\uparrow \downarrow}(t) = \frac{1}{2} \left( 1 \pm \text{Re}[\langle \psi^\uparrow(t_f) | \psi \uparrow(t_f) \rangle] \right).
\]  

In the case of maximal visibility \( |\langle \psi^\uparrow(t_f) | \psi \uparrow(t_f) \rangle| = 1 \), which can be realized using STA-mediated guided interferometry \[16\], the populations are given by

\[
P_{\uparrow \uparrow}(t) = \frac{1}{2} \left( 1 \pm \cos[\Delta \phi(t_f)] \right).
\]

In case the differential phase is proportional to a constant force \( F_0 \) [i.e. \( \Delta \phi(t_f) = SF_0 \)], \( F_0 \) can be determined from the populations provided that the sensitivity \( S \) is known. Importantly, in the envisaged scheme for force measurements the differential phase does not depend on the initial atomic motional state, hence it is not necessary to prepare atoms in their perfect ground state. This speaks in favor of the flexibility of the proposed scheme.

Having described the basics of the proposed interferometric scheme for constant-force measurements, we now point out the reasons as to why DWOLs should be eminently suitable for its experimental implementation. Firstly, spin-dependent DWOLs were demonstrated soon after the original realization of this type of optical lattices \[19\]. Secondly, the optical potential of DWOLs has an unusual property, highly beneficial in this context. Namely, the expansion of this potential in the \( x \)-direction, up to quadratic order, contains a nonzero term linear in \( x \) [cf. Eq. \[12\]], a property that sets DWOLs apart from conventional (single-well) optical lattices. As a result, the Hamiltonian governing the interferometer between the two \( \pi/2 \) pulses (i.e. the one describing the splitting and recombination parts of the interferometric sequence), which in the generic situation would contain the term \(-F_0 x\), in the case of DWOLs involves a different term linear in \( x \). The modified linear term is given by \(-\tilde{F}_0 x\), with \( \tilde{F}_0 \equiv F_0 + ma_x \), with \( a_x \) being proportional to the optical-potential amplitude \( U_{d,0} \) [cf. Eq. \[13\]].

In other words, the proposed force-measurement method in the case of DWOLs can be seen as a procedure for extracting the value of \( \tilde{F}_0 \), given by a sum of the sought-after force \( F_0 \) and a constant offset term \( ma_x \), which – being proportional to \( U_{d,0} \) – can be made rather large. This, in turn, drastically reduces the relative error in the experimental measurement of the unknown constant force. Therefore, the use of DWOLs should allow much more accurate measurements of constant homogeneous forces than conventional (single-well) optical lattices.

VIII. SUMMARY AND CONCLUSIONS

To summarize, in this paper we investigated coherent single-atom transport in a double-well optical lattice, a system characterized by a nonseparable optical potential in the \( x - y \) plane. We first proposed specific configurations of acousto-optic modulators that give rise to the moving-lattice effect in this system, thus enabling atom transport in an arbitrary direction. We then designed appropriate moving-lattice trajectories using both shortcuts to adiabaticity (STA) and their recently proposed enhanced version, known as eSTA. Through numerical solution of the time-dependent Schrödinger equation in the comoving frame, based on the previously obtained STA and eSTA moving-lattice trajectories, we evaluated the efficiency of the resulting single-atom transport as quantified by the transport fidelity.

We showed that – while the STA method enables somewhat faster transport in shallow double-well optical lattices (i.e. for small lattice depths) – the eSTA method outperforms it consistently for sufficiently deep lattices (more precisely, for lattice depths above around hundred recoil energies). We also identified the atom-transport implications of the specific geometric structure of double-well optical lattices, as well as of their characteristic spatial anisotropy. In addition, we discussed the implications of the proposed transport schemes in neutral-atom quantum computing, i.e. the realization of collisional two-qubit entangling gates. Finally, we pointed out that guided-atom interferometry enabled by spin-dependent transport in double-well optical lattices may allow accurate measurements of constant homogeneous forces, an important application in the realm of quantum sensing.

In contrast to most previous theoretical studies of coherent single-atom transport, which were based on simplified scenarios, in the present paper we investigated this phenomenon based on the full, nonseparable double-well optical potential. Therefore, the results we obtained can be corroborated in future atom-transport experiments in such lattices. Moreover, our study also complements nicely the recent body of work on quantum-state control of Bose-Einstein condensates in optical lattices \[36\] \[37\]. Finally, our work may motivate further attempts to realistically model single-atom transport in complex optically-trapped neutral-atom systems, including those that could potentially be based on the recently proposed formalism of open-system STA \[22\].

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Appendix A: Derivation of the expression for \( G_n \)

In what follows, we derive an expression that can be used as the basis for the evaluation of the first (scalar) auxiliary function \( G_n \) [cf. Eq. (35)] in the problem at hand. For the sake of brevity, the multi-indices \( \mathbf{n} \equiv (n_x, n_y, n_z) \) and \( \mathbf{n}_r \equiv (n_x, n_y) \) are used.

The transport modes (for transport within the \( x - y \) plane) of our simplified DWOL Hamiltonian \( H_{DOL}(t) \) [cf. Eq. (23)], which has the form characteristic of a 3D harmonic oscillator, in the coordinate representation are given by

\[
\langle \mathbf{r} | \Psi_n \rangle = \exp \left[ -\frac{i}{\hbar} \left( E_n t + \frac{m}{2} \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp \left[ i \left( \frac{\omega_x n_x + \omega_z n_z}{l_x \sqrt{2}} \right) x \right] \exp \left[ -\frac{\omega_x^2 n_x^2 + \omega_z^2 n_z^2}{2 l_x^2} \right] \right] \right] \exp \left[ (i m \omega_x n_x t + \frac{\pi}{2 l_x}) H_{n_x} \left( \frac{x - q_{c,x}(t)}{l_x \sqrt{2}} \right) H_{n_y} \left( \frac{y - q_{c,y}(t)}{l_y \sqrt{2}} \right) H_{n_z} \left( \frac{z}{l_z \sqrt{2}} \right) \right] (A1)
\]

where \( E_n = \hbar \omega_x (n_x + 1/2) + \hbar \omega_y (n_y + 1/2) + \hbar \omega_z (n_z + 1/2) - m a_z^2 / (2 l_x^2) \) is the \( n \)-th energy eigenvalue and \( l_j \equiv \sqrt{\hbar / (2 m \omega_j)} \) is the characteristic length scale along the direction \( j \) (\( j = x, y, z \)). The energies \( E_n \) contain a constant-energy offset due to the presence of a linear term in \( x \) in the approximated potential of Eq. (12).

By inserting these last transport modes of a 3D harmonic Hamiltonian into Eq. (60), we obtain

\[
G_n = \int_0^t dt \int_{-\infty}^{\infty} dZ \int_{-\infty}^{\infty} dY \int_{-\infty}^{\infty} dX \exp \left[ i \left( \frac{\omega_x n_x + \omega_z n_z}{l_x \sqrt{2}} \right) x \right] \exp \left[ -\frac{\omega_x^2 n_x^2 + \omega_z^2 n_z^2}{2 l_x^2} \right] \right] \exp \left[ (i m \omega_x n_x t + \frac{\pi}{2 l_x}) H_{n_x} \left( \frac{x - q_{c,x}(t)}{l_x \sqrt{2}} \right) H_{n_y} \left( \frac{y - q_{c,y}(t)}{l_y \sqrt{2}} \right) H_{n_z} \left( \frac{z}{l_z \sqrt{2}} \right) \right] (A2)
\]

In the equation above, we introduced the dimensionless coordinates \( X = x / (l_x \sqrt{2}) \), \( Y = y / (l_y \sqrt{2}) \), \( Z = z / (l_z \sqrt{2}) \) and new functions \( X_0(t) := X - q_{c,x}(t) / (l_x \sqrt{2}) \), \( Y_0(t) := Y - q_{c,y}(t) / (l_y \sqrt{2}) \), \( X_C(t) := X - \tilde{q}_{c,x}(t) / (l_x \sqrt{2}) \) and \( Y_C(t) := Y - \tilde{q}_{c,y}(t) / (l_y \sqrt{2}) \). The displaced classical path of the potential minima \( \tilde{q}_{c,x/y}(t) = q_{c,x/y}(t) - \pi / (2 l_x) \) was introduced into the above equation to simplify the upcoming integrations. The general solution of Eq. (A2) will be obtained by treating the different terms and integrations separately from each other.

1. “Out-of-plane” integration

The integration will be started by considering the relatively simple calculation along the \( z \) direction. Since the full \( Z \)-dependent integration cannot be done with \( Z \)-dependent waists, we will use the approximation

\[
\sqrt{1 + \left( \frac{Z l_x}{Z_{R,u}} \right)^2} \approx 1 \quad (u = x, y), \quad (A3)
\]

valid for \( Z_{R,u} \gg l_z \). The approximation above can straightforwardly be verified by comparing the scales on which the exponential function and the waists change significantly. Ordering the different terms in Eq. (A2) results in the integral

\[
I_{n_z}^{DOL} = \int_{-\infty}^{\infty} dZ H_{n_z}(Z) \exp (-Z^2) \left[ A + 2 B \cos^2(\sqrt{2} k_z Z l_z) + C \cos(\sqrt{2} k_z Z l_z) + D Z^2 \right], \quad (A4)
\]

with the prefactors \( A, B, C, D \), which themselves can be identified with \( x \)- and \( y \)-dependent terms from Eq. (A2). For the sake of readability, we refrain from explicitly writing down the long expressions for these prefactors.
To calculate the above integral we restrict ourselves to the integration of a simplified integral, given by

\[ I_{n_{x,1}}^{m} = \int_{-\infty}^{\infty} dZ H_n(z) \exp \left( -Z^2 \right) \cos^{2} \left( \sqrt{2} k l_x Z \right) \]

\[ = \frac{1}{4} \sum_{k_1 + 2k_2 = n_x} \frac{n_{x}}{k_1!k_2!}(-1)^{k_1+k_2} 2^{k_1} \int_{-\infty}^{\infty} dZ Z^{k_1} \exp \left( -Z^2 \right) \left[ \exp \left( i 2^{3/2} k l_x Z \right) + \exp \left( -i 2^{3/2} k l_x Z \right) + 2 \right]. \]

(A5)

In the above calculations, use has been made of the Faà di Bruno representation of Hermite polynomials \[86\]

\[ H_m(x) = (-1)^m \sum_{k_1 + 2k_2 = m} \frac{m!}{k_1!k_2!}(-1)^{k_1+k_2} (2x)^{k_1}. \]

(A6)

The integral in Eq. (A5) can be calculated by ordering the different terms and making use of the following result:

\[ \int_{-\infty}^{\infty} dx x^n \exp \left( -a x^2 + b x + c \right) = \exp \left( \frac{b^2}{4a} + c \right) \sum_{k=0}^{[n/2]} \left( \frac{n}{2k} \right) \left( \frac{b}{2a} \right)^{n-2k} \Gamma \left( k + 1/2 \right). \]

(A7)

Therefore, we just state the final result, which is given by

\[ I_{n_{x,1}}^{m} = \frac{1}{4} \sum_{k_1 + 2k_2 = n_x} \frac{n_{x}}{k_1!k_2!}(-1)^{k_1+k_2} 2^{k_1} \sum_{\lambda=0}^{[k_1/2]} \left( \frac{k_1}{2\lambda} \right) \Gamma \left( \lambda + 1/2 \right) \exp \left( -2 k^2 l_x^2 \right)
\times \left[ \left( i 2^{3/2} k l_x \right)^{k_1-2\lambda} + \left( -i 2^{3/2} k l_x \right)^{k_1-2\lambda} + 2 \delta_{k_1,2\lambda} \right]. \]

(A8)

With the above solution it is straightforward to complete the evaluation of the integral in Eq. (A4). Thus, we just state the final result

\[ I_{n_{x}}^{D} = (A + B) \sqrt{\pi} \delta_{n_{x},0} + \frac{B}{2} \left( 2^{3/2} i k_x l_x \right)^{n_x} \exp \left( -2 k_x^2 l_x^2 \right) \sqrt{\pi} \delta_{n_{x},N_{g}}
\times \frac{C}{2} \left( i \sqrt{2} k_x l_x \right)^{n_x} \exp \left( -\frac{k_x^2}{2} l_x^2 \right) \sqrt{\pi} \delta_{n_{x},N_{g}} + D \sqrt{\pi} \left( \frac{1}{2} \delta_{n_{x},0} + 2 \delta_{n_{x},2} \right), \]

(A9)

where \( N_{g} \) stands for the set of even positive integers.

2. **“In-plane” integration**

In the following we consider integrals over the \( x \) coordinate. The corresponding integrals in \( y \) can straightforwardly be evaluated in an analogous manner i.e. by replacing the parameters for the \( x \) components of the potentials, such as \( q_{c.x}(t) \) and \( q_{0.x}(t) \), with their \( y \)-coordinate counterparts.

The first integral to be considered is given by

\[ I_{n_{x}}^{D} (k_x, t) = \int_{-\infty}^{\infty} dX H_{n_{x}} \left[ X_{C}(t) \right] \exp \left[ -X_{C}^{2}(t) \right] \cos \left[ 2^{3/2} k_x l_x X_{0}(t) \right] \]

(A10)

and can be computed by rewriting the cosine function in terms of exponential functions and making use of the Faà di Bruno representation of Hermite polynomials [cf. Eq. (A6)]. In this manner, the following solution is readily obtained:

\[ I_{n_{x}}^{D} (k_x, t) = (-1)^{n_x} \left( \frac{1}{2} \right) \sum_{k_1 + 2k_2 = n_x} \frac{n_{x}}{k_1!k_2!}(-1)^{k_1+k_2} 2^{k_1} \exp \left( -2 k_x^2 l_x^2 \right) \sum_{l=0}^{[k_1/2]} \left( \frac{k_1}{l} \right) \left[ \frac{\tilde{q}_{c.x}(t)}{\sqrt{2} l_x} \right]^{k_1-l}
\times \sum_{\lambda=0}^{[l/2]} \left( \frac{l}{2\lambda} \right) \Gamma \left( \lambda + 1/2 \right) \left\{ \exp \left( 2i k_x \left[ \tilde{q}_{c.x}(t) - q_{0.x}(t) \right] \right) \left[ \frac{\tilde{q}_{c.x}(t)}{\sqrt{2} l_x} + i \sqrt{2} k_x l_x \right]^{l-2\lambda} \right. \right.
\left. + \exp \left( -2i k_x \left[ \tilde{q}_{c.x}(t) - q_{0.x}(t) \right] \right) \left[ \frac{\tilde{q}_{c.x}(t)}{\sqrt{2} l_x} - i \sqrt{2} k_x l_x \right]^{l-2\lambda} \right\}. \]

(A11)
The sine-function counterpart of the integral in Eq. (A10) is readily obtained by following analogous steps. The final solution is given by

\[ I_{n_x}^{DS} (k_L, t) = \int_{-\infty}^{\infty} dX \frac{n_x}{X_c (t)} \exp \left[ X_c^2 (t) \right] \sin \left[ 2^{3/2} k_L X_c (t) \right] \]

\[ = (-1)^{n_x+1} \frac{1}{2} \sum_{k_1 + 2k_2 = n_x} \frac{n_x!}{k_1!k_2!} (-1)^{k_1+k_2} 2^{k_1} \sum_{l=0}^{k_1} \left( \frac{1}{2} \right) \left( \begin{array}{l} l \\ 2 \lambda \end{array} \right) \Gamma (\lambda + 1/2) \exp \left[ 2i k_L (\tilde{q}_{c,x} (t) - q_{0,x} (t)) \right] \frac{\tilde{q}_{c,x} (t)}{\sqrt{2} l_x} \right]^{1-2\lambda} \]

\[ \times \sum_{\lambda=0} \left( \begin{array}{l} l \\ 2 \lambda \end{array} \right) \Gamma (\lambda + 1/2) \frac{\tilde{q}_{c,x} (t)}{\sqrt{2} l_x} \right]^{1-2\lambda} \exp \left[ -2k_L^2 l_x^2 \right]. \]

(A12)

As was to be expected, the only differences with respect to Eq. (A11) are the change of sign in the brackets and the additional prefactor of \((-i)\).

Let us now consider the \(X_0(t)\)-dependent exponential term that appears within the potential used in Eq. (A12), for which we first evaluate the following integral:

\[ I_{n_x}^{DS} (t) = \int_{-\infty}^{\infty} dX \frac{n_x}{X_c (t)} \exp \left[ X_c^2 (t) \right] \exp \left[ -\frac{X_0^2 (t) l_x^2}{w_{0,x}^2} \right] \]

\[ = \int_{-\infty}^{\infty} dX \frac{n_x}{X_c (t)} \exp \left[ X_c^2 (t) \right] \exp \left[ -\frac{X_0^2 (t) l_x^2}{w_{0,x}^2} \right] \exp \left[ -\left( 1 + \frac{4l_x^2}{w_{0,x}^2} \right) X_c^2 \right] \]

\[ \times \exp \left[ \frac{\tilde{q}_{c,x} (t)}{2l_x} + 2q_{0,x} (t) \right] \frac{l_x}{2} \sqrt{2} X_c \exp \left[ -\frac{\tilde{q}_{c,x} (t)}{2l_x} - \frac{2q_{0,x} (t)}{w_{0,x}^2} \right]. \]

(A13)

Up until this point we ordered the terms in the argument of the exponential function in terms of a polynomial in \(X_c\) and used the identity

\[ H_m (x + y) = \sum_{k=0}^{m} \binom{m}{k} H_k (x) (2y)^{m-k} \]

(A14)

to separate the terms in the argument of the Hermite polynomial. Now we are able to use the integral relation of Eq. (A7), along with the Faà di Bruno representation of Hermite polynomials [cf. Eq. (A10)], to obtain the following result:

\[ I_{n_x}^{DS} (t) = \sum_{\lambda=0}^{n_x} \binom{n_x}{\lambda} \sum_{k_1 + 2k_2 = \lambda} (-1)^{n_x+k_1+k_2} \frac{\lambda!}{k_1!k_2!} 2^{k_1} \exp \left[ -2 \frac{q_{0,x} (t) - q_{c,x} (t)}{4l_x^2 + w_{0,x}^2} \right] \]

\[ \times \left[ \sqrt{2} \tilde{q}_{c,x} (t) \right] \sum_{\sigma=0}^{k_1-1} \left( \begin{array}{l} k_1 \\ 2 \sigma \end{array} \right) \left[ \frac{4l_x^2 q_{0,x} (t) - \tilde{q}_{c,x} (t) w_{0,x}^2}{2^{5/2} l_x^3 + \sqrt{2} l_x w_{0,x}^2} \right] \left[ 1 + \frac{4l_x^2}{w_{0,x}^2} \right]. \]

(A15)

The terms in Eq. (A2) that originate from the contribution \(\tilde{U}_{cs}\) to the full DWOL potential [cf. Eq. (10)] result in the same integral as in Eq. (A13) above but with an additional \(X_0(t)\)-dependent cosine term and without a factor of two in the argument of the exponential function:

\[ I_{n_x}^{DS} (t) = \int_{-\infty}^{\infty} dX \frac{n_x}{X_c (t)} \cos \left[ \sqrt{2} k_L X_0 (t) l_x \right] \exp \left[ -X_c^2 (t) \right] \exp \left[ -2 \frac{X_0^2 (t) l_x^2}{w_{0,x}^2} \right]. \]

(A16)
By repeating analogous steps as in the derivation of Eq. (A15), we obtain the following solution:

$$I_{n_x}^{D^3}(t) = \frac{1}{2} \sum_{\lambda=0}^{n_x} (-1)^{\lambda} \left( \frac{n_x}{\lambda} \right) \sum_{k_1+k_2=\lambda} (-1)^{k_1+k_2} \frac{\lambda!}{k_1!k_2!} 2^{k_1} \left[ -\sqrt{2} \hat{g}_{c,x}(t) \right]^{n_x-\lambda}$$

$$\times \exp \left( \frac{4 \left[ q_0(t)x - \hat{q}_{c,x}(t) \right]^2 + 2 k_1^2 L_x^2 w_{0,x}^2}{4 \left( 2 l_x^2 + w_{0,x}^2 \right)} \right) \sum_{\sigma=0}^{\lfloor k_1/2 \rfloor} \left( \frac{k_1}{2\sigma} \right) \frac{\Gamma (\sigma + 1/2)}{(1 + \frac{4 k_1^2 w_{0,x}^2}{w_{0,x}^2})^{\sigma+1/2}}$$

$$\times \left\{ \exp \left( -i k_L \left[ q_0(t)x - \hat{q}_{c,x}(t) \right] w_{0,x}^2 \left( 2 l_x^2 + w_{0,x}^2 \right) \right) \left[ \frac{2 l_x q_0(t)x}{w_{0,x}^2} + i k_L l_x + \hat{q}_{c,x}(t) l_x \right] \sqrt{2} \left( 1 + \frac{2 k_1^2 w_{0,x}^2}{w_{0,x}^2} \right) \right\} k_1 - 2\sigma \right)$$

(A17)

The next step is to consider the integral similar to the one discussed above, in which the cosine is substituted by a sine function. The integral in question is given by

$$I_{n_x}^{D^3^S}(t) = \int_{-\infty}^{\infty} dX H_{n_x} [X_C(t)] \sin \left[ \sqrt{2} k_L X_0(t) l_x \right] \exp \left[ -X_0^2(t) \right] \exp \left( -2 \frac{X_0^2(t) L_x^2}{w_{0,x}^2} \right).$$

(A18)

By repeating similar steps as in the derivation of Eq. (A17), we obtain the solution of the last integral in the following form:

$$I_{n_x}^{D^3^S}(t) = \int_{-\infty}^{\infty} dX H_{n_x} [X_C(t)] \sin \left[ \sqrt{2} k_L X_0(t) l_x \right] \exp \left[ -X_0^2(t) \right] \exp \left( -2 \frac{X_0^2(t) L_x^2}{w_{0,x}^2} \right)$$

$$= \frac{i}{2} \sum_{\lambda=0}^{n_x} (-1)^{\lambda+1} \left( \frac{n_x}{\lambda} \right) \sum_{k_1+k_2=\lambda} (-1)^{k_1+k_2} \frac{\lambda!}{k_1!k_2!} 2^{k_1} \left[ -\sqrt{2} \hat{g}_{c,x}(t) \right]^{n_x-\lambda}$$

$$\times \exp \left( -2 \frac{\left[ q_0(t)x - \hat{q}_{c,x}(t) \right]^2 + k_1^2 l_x^2 w_{0,x}^2}{2 \left( 2 l_x^2 + w_{0,x}^2 \right)} \right) \sum_{\sigma=0}^{\lfloor k_1/2 \rfloor} \left( \frac{k_1}{2\sigma} \right) \frac{\Gamma (\sigma + 1/2)}{(1 + \frac{4 k_1^2 w_{0,x}^2}{w_{0,x}^2})^{\sigma+1/2}}$$

(A19)

$$\times \left\{ \exp \left( -i k_L \left[ q_0(t)x - \hat{q}_{c,x}(t) \right] w_{0,x}^2 \left( 2 l_x^2 + w_{0,x}^2 \right) \right) \left[ \frac{2 l_x q_0(t)x}{w_{0,x}^2} + i k_L l_x + \hat{q}_{c,x}(t) l_x \right] \sqrt{2} \left( 1 + \frac{2 k_1^2 w_{0,x}^2}{w_{0,x}^2} \right) \right\} k_1 - 2\sigma \right)$$

The integration over the $\theta$-dependent trigonometric function emergent through the potential of Eq. (A2) can straightforwardly be carried out using the following familiar identity:

$$\sin \left[ \sqrt{2} k_L l_x X_0(t) - \theta \right] = \sin \left[ \sqrt{2} k_L l_x X_0(t) \right] \cos \theta - \cos \left[ \sqrt{2} k_L l_x X_0(t) \right] \sin \theta.$$

(A20)

Thus, the integral can be reduced to the integrals involving trigonometric functions that were already evaluated above [cf. Eq. (A11) and (A12)].

The integration involving the $X_0^2(t)$-dependent terms of Eq. (A2) can be carried out by making use of the identity

$$x H_m(x) = \frac{1}{2} H_{m+1}(x) + m H_{m-1}(x),$$

(A21)
as well as the orthogonality of Hermite polynomials. Thus, the integral in $X$ is given by

$$I_{n,x}^{D4}(t) = \frac{\hbar \omega_x}{2} \int_{-\infty}^{\infty} dX \exp \left[ -X^2 \right] X_0^2(t) H_{n_x} [X_C(t)] \delta_{n_x,0} \delta_{n_y,0}$$

$$= \frac{\hbar \omega_x}{2} \int_{-\infty}^{\infty} dX \sum_{m=0}^{\infty} \frac{H_m(X)}{m!} \left[ \frac{\tilde{q}_{c,x}(t)}{\sqrt{2} l_x} \right]^m \exp \left( -X^2 \right) \delta_{n_x,0} \delta_{n_y,0}$$

$$\times \left[ X^2 - \sqrt{2} X \frac{q_0_X(t)}{l_x} + \frac{\tilde{q}_{c,x}(t)}{2 l_x^2} \right] \sum_{l=0}^{n_x} \left( \frac{n_x}{l} \right)_l \left( \frac{n_x}{l} \right)_{n_x-l} H_l(X) \left[ -\sqrt{2} \frac{\tilde{q}_{c,x}(t)}{l_x} \right]^{n_x-l}$$

$$= \frac{\hbar}{2} \sqrt{\pi} \omega_x \delta_{n_x,0} \delta_{n_y,0} \left[ \frac{\sqrt{2} \tilde{q}_{c,x}(t)}{l_x} \right]^{n_x}$$

$$\times \sum_{l=0}^{n_x} \left( \frac{n_x}{l} \right) (-1)^{n_x-l} \left\{ \frac{1}{4} l(l-1) \left[ \frac{\tilde{q}_{c,x}(t)}{\sqrt{2} l_x} \right]^{-2} - l q_0_X(t) \tilde{q}_{c,x}(t)^{-1} + l \right\},$$

(A22)

where we have made use of the binomial theorem and the condition $n > 0$. The final expression for the above integral is given by

$$I_{n,x}^{D4}(t) = \frac{\hbar}{2} \omega_x \int_{-\infty}^{\infty} dX \exp \left[ -X^2 \right] X_0^2(t) H_{n_x} [X_C(t)] \delta_{n_x,0} \delta_{n_y,0}$$

$$= \hbar \omega_x \sqrt{\pi} \delta_{n_x,0} \delta_{n_y,0} \left[ \delta_{n_x,1} \tilde{q}_{c,x}(t) - q_0_X(t) \right] + \delta_{n_x,2}.$$  

(A23)

The last term that we need to integrate is the term linear in $X_0(t)$. The corresponding solution can straightforwardly be obtained through the following evaluation:

$$I_x^c = \int_{-\infty}^{\infty} dX \exp \left[ -X^2 \right] X_0(t) H_{n_x} [X_C(t)] \delta_{n_x,0} \delta_{n_y,0}$$

$$= \int_{-\infty}^{\infty} dX \sum_{m=0}^{\infty} \frac{1}{m!} \left[ \frac{\tilde{q}_{c,x}(t)}{\sqrt{2} l_x} \right]^m \sum_{l=0}^{n_x} \left( \frac{n_x}{l} \right)_l H_l(X) \left[ -\sqrt{2} \frac{\tilde{q}_{c,x}(t)}{l_x} \right]^{n_x-l}$$

$$\times \left[ \frac{1}{2} H_{m+1}(X) - \frac{q_0_X(t)}{\sqrt{2} l_x} H_m(X) + m H_{m-1}(X) \right] \exp \left( -X^2 \right) \delta_{n_x,0} \delta_{n_y,0}$$

(A24)

$$= \sqrt{\pi} \delta_{n_x,0} \delta_{n_y,0} \left[ \frac{\sqrt{2} \tilde{q}_{c,x}(t)}{l_x} \right]^{n_x-1} \sum_{l=0}^{n_x} \left( \frac{n_x}{l} \right) (-1)^{n_x-l},$$

where use has been made of the same steps utilized above for the evaluation of the integral in Eq. (A23). Using mathematical induction it can further be demonstrated that only contributions with $n_x = 1$ are not equal to zero. Thus, the final result reads

$$I_x^c = \sqrt{\pi} \delta_{n_x,1} \delta_{n_y,0} \delta_{n_x,0}.$$  

(A25)

Putting the different solutions for the integrals of Eq. (A20) together and using the orthogonality of Hermite polynomials, the first auxiliary function can be reduced to the time integral

$$G_n = -\int_0^{\mathcal{T}} dt \frac{U_{d,0}}{2} \frac{\exp \left[ i \left( \omega_x n_x + \omega_y n_y + \omega_z n_z \right) t \right]}{2^{n_x} n_x! n_y! n_z! \pi^2}$$

$$\left\{ \zeta_{||,n}(t) + \zeta_{\perp,n}(t) + \zeta_{z,n}(t) + \zeta_{c,r,n}(t) \right\}$$

$$+ \hbar \sqrt{\pi} \frac{U_{d,0}}{\omega_x} \delta_{n_x,0} \delta_{n_y,0} \left[ \delta_{n_x,1} \frac{\tilde{q}_{c,x}(t) - q_0_X(t)}{\sqrt{2} l_x} + \delta_{n_x,2} \right]$$

$$+ \omega_x \left[ \frac{1}{2} \delta_{n_x,0} + 2 \delta_{n_x,2} \right] + \frac{1}{\sqrt{2} U_{d,0}} \left( 2 m a_x l_x + \hbar \omega_x \frac{k_{1,1}^{-1}}{2 l_x} \right) \pi \delta_{n_x,1} \delta_{n_y,0} \delta_{n_z,0}.$$  

(A26)
where $\zeta_{\|,n}(t)$, $\zeta_{\perp,n}(t)$, $\zeta_{x,n}(t)$, and $\zeta_{cr,n}(t)$ are functions of time given by:

$$\zeta_{\|,n}(t) = \cos^2 \left( \frac{\beta}{2} \right) \left[ I_{n_{x}}^{D} (k_{L}, t) \delta_{n_{x},0} - I_{n_{x}}^{D} (k_{L}, t) \delta_{n_{x},0} \right] \delta_{n_{x},0},$$

$$\zeta_{\perp,n}(t) = \sin^2 \left( \frac{\beta}{2} \right) \left[ I_{n_{x}}^{D} (k_{L}, t) \delta_{n_{x},0} - \cos (2\theta) I_{n_{x}}^{D} (k_{L}, t) \delta_{n_{x},0} + \frac{4}{\sqrt{\pi}} I_{n_{x}}^{D} (k_{L}, t/2, t) \left[ \sin \theta I_{n_{x}}^{D} (k_{L}/2, t) \right. \right.$$

$$- \cos \theta I_{n_{x}}^{DS} (k_{L}/2, t) \left. \right] - I_{n_{x}}^{DS} (k_{L}, t) \sin (2\theta) \delta_{n_{x},0} \right] \delta_{n_{x},0},$$

$$\zeta_{x,n}(t) = \frac{\xi_{\mu}}{\sqrt{\pi}} I_{n_{x}}^{D_{2}} (t) I_{n_{y}}^{D_{2}} (t) \left[ \frac{1}{2} \delta_{n_{x},0} + 2 \left( 2^{3/2} i k_{z} l_{z} \right)^{n_{x}} \exp \left( -2 \frac{k_{z}^{2} l_{z}^{2}}{2} \right) \delta_{n_{x},n_{y}} \right],$$

$$\zeta_{cr,n}(t) = 2 \sqrt{\frac{\xi_{\mu}}{\pi}} \cos \left( \frac{\beta}{2} \right) \cos \left( \phi \right) \left[ I_{n_{x}}^{D_{2}} (t) I_{n_{y}}^{D_{3}} (t) - \sin \left( \phi \right) I_{n_{x}}^{D_{3S}} (t) I_{n_{y}}^{D_{2}} (t) \right] \left( i \sqrt{2} k_{x} l_{x} \right)^{n_{x}} \exp \left( -2 \frac{k_{x}^{2} l_{x}^{2}}{2} \right) \delta_{n_{x},n_{y}} \right].$$

(A27)

The evaluation of the time integral in Eq. (A26), the last step in the calculation of the first auxiliary function $G_{n}$, can only be done numerically.

Appendix B: Derivation of the expression for $K_{n}$

In the following, we express an expression that can be used as the basis for a numerical evaluation of the second (vector) auxiliary function $K_{n}$ [cf. Eq. (B3)] in the problem at hand.

To derive the desired expression for $K_{n}$, the gradient with respect to $\lambda$, and subsequently to $\alpha$, of the Hamiltonian $H_{DW}$ is needed. Since the differentiations are straightforward, we just state the resulting equation for $K_{n}$:

$$K_{n} = \int_{0}^{t_{1}} dt \int_{-\infty}^{\infty} dZ \int_{-\infty}^{\infty} dY \int_{-\infty}^{\infty} dX \frac{1}{\sqrt{2n_{x}!n_{y}!n_{z}!n_{z}!}} \exp \left[ i \left( n_{x} \omega_{x} + n_{y} \omega_{y} + n_{z} \omega_{z} \right) t \right]$$

$$\times H_{n_{x}} \left[ X_{C}(t) \right] H_{n_{y}} \left[ Y_{C}(t) \right] H_{n_{z}} \left[ Z(t) \right] \exp \left[ -X_{C}^{2}(t) \right] \exp \left[ -Y_{C}^{2}(t) \right] \exp \left[ -Z^{2}(t) \right] \] $$

$$\times \left[ \frac{\omega_{x}^{2}}{\sqrt{2}} X_{0}(t) l_{x}, \frac{\omega_{y}^{2}}{\sqrt{2}} Y_{0}(t) l_{y}, \frac{\omega_{z}^{2}}{\sqrt{2}} Z(t) l_{z} \right] \bigg|_{\alpha=0}.$$

We start by noting that the integral over $Z$ has the same general form as Eq. (A14) and, accordingly, the same solution that is given by Eq. (A9). In fact, most of the needed integrals have already been carried out in the evaluation of the first auxiliary function (cf. Appendix A). Even the cosine term originating from the potential in Eq. (B1) can be rewritten using the trigonometric identity

$$\cos \left[ \sqrt{2} k_{l} l_{x} X_{0}(t) - \theta \right] = \cos \left[ \sqrt{2} k_{l} l_{x} X_{0}(t) \right] \cos \theta + \sin \left[ \sqrt{2} k_{l} l_{x} X_{0}(t) \right] \sin \theta,$$

(B2)

using which we can evaluate the relevant integrals by making use of the solutions in Eq. (A11) and Eq. (A12).

However, there are integrals that originate from the influence of the laser in the $z$ direction, which have not been considered previously. The first one among those integrals is given by

$$\bar{I}_{n_{x}}^{D_{2}} (t) = \int_{-\infty}^{\infty} dX X_{0}(t) H_{n_{x}} \left[ X_{C}(t) \right] \exp \left[ -X_{C}^{2}(t) \right] \exp \left[ -4 \frac{X_{0}^{2}(t) l_{x}^{2}}{\omega_{0,x}^{2}} \right]$$

$$= \int_{-\infty}^{\infty} dX \sum_{\lambda=0}^{n_{x}} \left( \frac{n_{x}}{\lambda} \right) H_{\lambda} (X) \left[ \sqrt{2} \frac{\bar{q}_{c,x}(t)}{l_{x}} \right]^{n_{x}-\lambda} \exp \left[ - \left( 1 + \frac{4l_{x}^{2}}{\omega_{0,x}^{2}} \right) X^{2} \right]$$

$$\times \left[ X - \frac{q_{0,x}(t)}{\sqrt{2} l_{x}} \right] \exp \left[ \left( \frac{\bar{q}_{c,x}(t)}{2l_{x}} + \frac{q_{0,x}(t)}{2\omega_{0,x}^{2}} l_{x} \right) \sqrt{2} X \right] \exp \left[ \frac{\bar{q}_{c,x}(t)}{2l_{x}^{2}} + \frac{q_{0,x}(t)}{2\omega_{0,x}^{2}} l_{x} \right]$$

$$= \sum_{\lambda=0}^{n_{x}} \left( \frac{n_{x}}{\lambda} \right) \sum_{k_{1}+2k_{2}=\lambda} \left( -1 \right)^{k_{1}+k_{2}} \left( \frac{l_{x}}{k_{1}^{1/2} l_{x}^{2}} \right) \left[ \sqrt{2} \frac{\bar{q}_{c,x}(t)}{l_{x}} \right]^{n_{x}-\lambda}$$

$$\times \exp \left[ - \left( \frac{2q_{0,x}(t) - \bar{q}_{c,x}(t)}{2^{3/2} l_{x}^{3} + \omega_{0,x}^{2}} \right)^{2} \right] \left[ D_{n_{x}} (k_{1} + 1, t) - \frac{q_{0,x}(t)}{\sqrt{2} l_{x}} D_{n_{x}} (k_{1}, t) \right],$$

(B3)
where use was made of the integral- and Hermite-polynomial identities in Eqs. (A.7) and (A.15), as well as the following function:

\[ \hat{D}_{n_+} (k, t) = \sum_{\sigma = 0}^{[k/2]} \left( \frac{k}{2\sigma} \right) \left[ \frac{4l_2^2 q_{0,x}(t) + \tilde{q}_{c,x}(t) w_{0,x}^2}{\sqrt{2} l_x \left( 4l_x^2 + w_{0,x}^2 \right)} \right]^{-2\sigma} \frac{\Gamma (\sigma + 1/2)}{\left( 1 + \frac{4l_x^2}{w_{0,x}^2} \right)^{\sigma + 1/2}}. \]  

(B4)

The integrations corresponding to the cross terms lead to the following final expressions:

\[ \hat{I}_{n_+}^{(3)} (k_L, t) = \int_{-\infty}^{\infty} dX n_{\pm} \left[ X_C(t) \right] X_0(t) \cos \left[ \sqrt{2} k_L X_0(t) l_x \right] \exp \left[ -X_0^2(t) \right] \exp \left[ -4 \frac{X_0^2(t) l_x^2}{w_{0,x}^2} \right] \]

\[ = \frac{1}{2^{3/2}} \int_{-\infty}^{\infty} dX \sum_{\lambda = 0}^{n_x} \left( \frac{n_x}{\lambda} \right) H_\lambda (X) \left[ -\sqrt{2} \tilde{q}_{c,x}(t) l_x \right]^{-n_x - \lambda} \exp \left[ -\left( 1 + \frac{4l_x^2}{w_{0,x}^2} \right) X^2 \right] \]

\[ \times \left[ X - \frac{q_0(t)}{\sqrt{2} l_x} \right] \exp \left( \frac{\tilde{q}_{c,x}(t)}{2l_x} + 2q_{0,x}(t) \frac{l_x}{w_{0,x}^2} \right) \sqrt{2} X \exp \left[ -\left( \frac{2q_{0,x}(t)}{2l_x^2 - w_{0,x}^2} - \frac{2q_{0,x}(t)}{2l_x^2} \right) \right] \]

\[ \times \left[ \exp \left( i \sqrt{2} X - \frac{q_0(t)}{\sqrt{2} l_x} \right) k_L l_x \right] + \exp \left( -i \sqrt{2} \left[ X - \frac{q_0(t)}{\sqrt{2} l_x} \right] k_L l_x \right) \]

\[ = \frac{1}{2} \sum_{\lambda = 0}^{n_x} (-1)^\lambda \left( \frac{n_x}{\lambda} \right) \sum_{k_1 + k_2 = \lambda} (-1)^{k_1 + k_2} \frac{\lambda!}{k_1!k_2!} q_{0,x} l_x \left[ -\sqrt{2} \tilde{q}_{c,x}(t) l_x \right]^{-n_x - \lambda} \]

\[ \times \exp \left( -4 \frac{\tilde{q}_{0,x}(t) - \tilde{q}_{c,x}^2(t)}{2 \left( 4l_x^2 + w_{0,x}^2 \right)} \right) \frac{\hat{D}_{k+1}^2 (k_1 + 1, k_L, t) - \frac{q_0(t)}{\sqrt{2} l_x} \hat{D}_{k_1}^2 (k_1, k_L, t)}{2 l_x^2} \]  

(B5)

Similar results are obtained by substituting the cosine with a sine in Eq. (B5):

\[ \hat{I}_{n_+}^{(3) S} (k_L, t) = \int_{-\infty}^{\infty} dX n_{\pm} \left[ X_C(t) \right] X_0(t) \sin \left[ \sqrt{2} k_L X_0(t) l_x \right] \exp \left[ -X_0^2(t) \right] \exp \left[ -4 \frac{X_0^2(t) l_x^2}{w_{0,x}^2} \right] \]

\[ = -\frac{i}{2} \sum_{\lambda = 0}^{n_x} (-1)^\lambda \left( \frac{n_x}{\lambda} \right) \sum_{k_1 + k_2 = \lambda} (-1)^{k_1 + k_2} \frac{\lambda!}{k_1!k_2!} q_{0,x} l_x \left[ -\sqrt{2} \tilde{q}_{c,x}(t) l_x \right]^{-n_x - \lambda} \]

\[ \times \exp \left( -4 \frac{\tilde{q}_{0,x}(t) - \tilde{q}_{c,x}^2(t)}{2 \left( 4l_x^2 + w_{0,x}^2 \right)} \right) \frac{\hat{D}_{k+1}^2 (k_1 + 1, k_L, t) - \frac{q_0(t)}{\sqrt{2} l_x} \hat{D}_{k_1}^2 (k_1, k_L, t)}{2 l_x^2} \]  

(B6)

In order to be able to succinctly write the solutions of the last integrals, we have introduced the following function:

\[ \hat{D}_{\pm}^2 (k, k_L, t) = \sum_{\sigma = 0}^{[k/2]} \left( \frac{k}{2\sigma} \right) \frac{\Gamma (\sigma + 1/2)}{\left( 1 + \frac{4l_x^2}{w_{0,x}^2} \right)^{\sigma + 1/2}} \]

\[ \times \left\{ \exp \left( -\frac{ik_L \left[ q_{0,x}(t) - \tilde{q}_{c,x}(t) \right] w_{0,x}^2}{4l_x^2 + w_{0,x}^2} \right) \right\} \frac{4l_x^2 q_{0,x}(t) + ik_L l_x^2 w_{0,x}^2 + \tilde{q}_{c,x}(t) w_{0,x}^2}{\sqrt{2} l_x \left( 4l_x^2 + w_{0,x}^2 \right)} \]

\[ \pm \exp \left( \frac{ik_L \left[ q_{0,x}(t) - \tilde{q}_{c,x}(t) \right] w_{0,x}^2}{4l_x^2 + w_{0,x}^2} \right) \right\} \frac{4l_x^2 q_{0,x}(t) - ik_L l_x^2 w_{0,x}^2 + \tilde{q}_{c,x}(t) w_{0,x}^2}{\sqrt{2} l_x \left( 4l_x^2 + w_{0,x}^2 \right)} \]  

(B7)

Having completed all the necessary spatial integrals, we can finally express the second auxiliary function in the form of the time integral

\[ K_n = -\int_0^{t_f} dt \frac{2 U_{d_0 k_L}}{\sqrt{2} l_x n_x n_y n_z n_r} \exp \left[ i \left( n_x \omega_x + n_y \omega_y + n_z \omega_z + n_r \omega_r \right) \right] \left[ \tilde{\zeta}_{\parallel,n}(t) + \tilde{\zeta}_{\perp,n}(t) + \tilde{\zeta}_{x,n}(t) + \tilde{\zeta}_{r,n}(t) \right] \]  

(B8)
where \( \tilde{\zeta}_{||,n}(t) \), \( \tilde{\zeta}_{\bot,n}(t) \), and \( \tilde{\zeta}_{x,n}(t) \) are vector functions of time given by:

\[
\tilde{\zeta}_{||,n}(t) = \cos^2 \left( \frac{\beta}{2} \right) \delta_{n_x,0} \left[ \nabla_{\alpha} f_{y}(\alpha_y; t) I_{n_x}^{DS}(k_L, t) \delta_{n_x,0} - \nabla_{\alpha} f_{x}(\alpha_x; t) I_{n_x}^{DS}(k_L, t) \delta_{n_x,0} \right] \bigg|_{\alpha = 0},
\]

\[
\tilde{\zeta}_{\bot,n}(t) = 2 \delta_{n_x,0} \sin^2 \left( \frac{\beta}{2} \right) \left[ \nabla_{\alpha} f_{y}(\alpha_y; t) I_{n_x}^{DS}(k_L/2, t) \delta_{n_x,0} + \nabla_{\alpha} f_{x}(\alpha_x; t) I_{n_x}^{DS}(k_L/2, t) \delta_{n_x,0} \right] \bigg|_{\alpha = 0},
\]

\[
\tilde{\zeta}_{x,n}(t) = \frac{2^{3/2}}{k_L} \sqrt{\frac{\xi_{x}}{\pi}} \cos \left( \frac{\beta}{2} \right) \left[ \nabla_{\alpha} f_{x}(\alpha_x; t) \frac{l_x}{u_{0,x}} I_{n_x}^{DS}(t) I_{n_y}^{D2}(t) + \nabla_{\alpha} f_{y}(\alpha_y; t) \frac{l_y}{u_{0,y}} I_{n_y}^{DS}(t) I_{n_x}^{D2}(t) \right] \bigg|_{\alpha = 0}.
\]

(B9)

The remaining integral over time can only be evaluated numerically, similarly to the evaluation of the first auxiliary function \( G_n \) [cf. Eq. (A20) in Sec. A2],

Appendix C: Derivation of the expression for \( \hat{T}_{x,p}(\delta t) \)

In the following we derive the expression for \( \hat{T}_{x,p}(\delta t) \), defined in Eq. (50), using the Baker-Campbell-Hausdorff (BCH) formula and its special case known as the Weyl identity (21).

We start by noting that \( \hat{T}_{x,p}(\delta t) \) can be rewritten as a product of three terms, each of which involves the coordinate- and momentum operators corresponding to one spatial direction:

\[
\hat{T}_{x,p}(\delta t) = \hat{T}_{x,p_x}(\delta t) \hat{T}_{y,p_y}(\delta t) \hat{T}_{z,p_z}(\delta t).
\]

(C1)

Therefore, it is sufficient to derive the expression for one of these operators, for instance

\[
\hat{T}_{x,p_x}(\delta t) = \exp \left( -\frac{i}{\hbar} \left[ \frac{p_x^2}{2m} \delta t + \hat{x} \int_{t}^{t+\delta t} m\hat{q}_{0,x}(t') dt' \right] \right),
\]

(C2)

and the remaining two can be derived in an analogous fashion. By realizing that

\[
\int_{t}^{t+\delta t} \hat{q}_{0,x}(t') dt' = \hat{q}_{0,x}(t + \delta t) - \hat{q}_{0,x}(t),
\]

(C3)

and introducing \( \delta \hat{q}_{0,x}(t) \equiv \hat{q}_{0,x}(t + \delta t) - \hat{q}_{0,x}(t) \), Eq. (C2) can be rewritten more succinctly as

\[
\hat{T}_{x,p_x}(\delta t) = \exp \left( -\frac{i}{\hbar} \left[ \frac{p_x^2}{2m} \delta t + m\delta \hat{q}_{0,x}(t) \hat{x} \right] \right).
\]

(C4)
At this point, we invoke the BCH formula \[ e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{i}{2} [\hat{A}, \hat{B}] + \frac{1}{12} [\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{12} [\hat{B}, [\hat{B}, \hat{A}]] + \ldots }, \] (C5)

where the ellipses in the exponent on the RHS of the last equation indicate the higher-order repeated commutators of \( \hat{A} \) and \( \hat{B} \). In what follows, we will use the last formula for \( \hat{A} = -i\delta t (2m\hbar)^{-1} \hat{p}_x^2 \) and \( \hat{B} = -im\hbar^{-1} \delta \hat{q}_{0,x}(t) \hat{x} \).

We first make use of the fact that \( [\hat{p}_x^2, \hat{x}] = -2i\hbar \hat{p}_x \), and that, accordingly, \( [\hat{p}_x^2, [\hat{p}_x^2, \hat{x}]] = 0 \) and \( [\hat{x}, [\hat{x}, \hat{p}_x^2]] = -4\hbar^2 \).

Thus, we first find that 
\[
\{ 0 = \left[ \hat{p}_x, \hat{p}_x \right] = \hat{p}_x \hat{p}_x - \hat{p}_x \hat{p}_x \},
\]
which along with the basic commutator \([\hat{x}, \hat{p}_x] = i\hbar \) implies that the second-order commutators of \( \hat{A} \) and \( \hat{B} \) are given by \([\hat{A}, [\hat{A}, \hat{B}]] = 0 \) and \([\hat{B}, [\hat{B}, \hat{A}]] = -2i\hbar^{-1} \delta \hat{q}_{0,x}(t) \hat{x} \)^2. The fact that the last commutator does not depend on \( \hat{x} \) and \( \hat{p}_x \) has two important implications. Firstly, all higher-order commutators are equal to zero, therefore for our choice of operators \( \hat{A} \) and \( \hat{B} \) there are no additional terms in the exponent on the RHS of Eq. (C5). Secondly, the commutator \([\hat{B}, [\hat{B}, \hat{A}]] \) itself gives rise only to a time-dependent global phase factor of the kind that is immaterial for our treatment of atom transport [recall similar arguments used for dropping terms in Eq. (44) of Sec. VVC] and can henceforth be disregarded. Therefore, we have

\[
\hat{T}_{x,p_x}(\delta t) = \exp \left( -\frac{i}{\hbar} \frac{\hat{p}_x^2}{2m} \delta t \right) \exp \left[ -\frac{i}{\hbar} \frac{\delta \hat{q}_{0,x}(t)}{\hbar} \hat{x} \right] \exp \left( -\frac{1}{4\hbar^2} [\hat{p}_x^2, \hat{x}] \delta t \delta \hat{q}_{0,x}(t) \right). \tag{C6}
\]
which further reduces to

\[
\hat{T}_{x,p_x}(\delta t) = \exp \left( -\frac{i}{\hbar} \frac{\hat{p}_x^2}{2m} \delta t \right) \exp \left[ -\frac{i}{\hbar} \frac{\delta \hat{q}_{0,x}(t)}{\hbar} \hat{x} \right] \exp \left( -\frac{i}{2\hbar} \frac{\hat{p}_x \delta \hat{q}_{0,x}(t)}{\delta t} \right). \tag{C7}
\]

Our goal is to reverse the order of the last two exponential operators on the RHS of the last equation, such that we can group all the kinetic terms together. To this end, we make use of the Weyl identity \[ \left[ \hat{A}, \hat{B} \right] = i\hbar^{-1} \delta \hat{q}_{0,x}(t) \] (i.e., \([\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{B}, \hat{A}]] = 0 \)):

\[
e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B} + \frac{i}{2} [\hat{A}, \hat{B}]} \tag{C8}.
\]

By exchanging the operators \( \hat{A} \) and \( \hat{B} \), we also obtain

\[
e^{\hat{B}} e^{\hat{A}} = e^{\hat{A} + \hat{B} - \frac{i}{2} [\hat{A}, \hat{B}]} \tag{C9}.
\]

Finally, by comparing Eqs. (C8) and (C9), we find that for operators \( \hat{A} \) and \( \hat{B} \) that commute with their commutator, one has

\[
e^{\hat{B}} e^{\hat{A}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{i}{2} [\hat{A}, \hat{B}]} \tag{C10}.
\]

We utilize the last identity for the operators

\[
\hat{A} = -\frac{i m \delta \hat{q}_{0,x}(t)}{\hbar} \hat{x}, \tag{C11}
\]

\[
\hat{B} = -\frac{i \delta \hat{q}_{0,x}(t)}{2\hbar} \hat{p}_x, \tag{C12}
\]

whose commutator is given by \([\hat{A}, \hat{B}] = -im(2\hbar)^{-1} \delta t [\delta \hat{q}_{0,x}(t)]^2 \] \[ \] . The last commutator not only commutes with both \( \hat{A} \) and \( \hat{B} \), but also does not depend on the operators \( \hat{x} \) and \( \hat{p}_x \) and is therefore immaterial for our present purposes. Therefore, the order of the last two terms on the RHS of Eq. (C7) can be reversed at the expense of an unimportant global phase factor. Thus, we can finally recast Eq. (C7) as

\[
\hat{T}_{x,p_x}(\delta t) = \exp \left( -\frac{i}{\hbar} \frac{\hat{p}_x^2}{2m} \delta t \right) \exp \left[ -\frac{i}{2\hbar} \hat{p}_x \delta \hat{q}_{0,x}(t) \right] \exp \left( -\frac{1}{\hbar} m \delta \hat{q}_{0,x}(t) \hat{x} \right). \tag{C13}
\]

The generalization of the last result to three dimensions, i.e. recovering the full expression for \( \hat{T}_{r,p}(\delta t) \) based on Eq. (C1), is straightforward. We finally obtain

\[
\hat{T}_{r,p}(\delta t) = \exp \left( -\frac{i}{\hbar} \frac{\hat{p}_x^2}{2m} \delta t \right) \exp \left[ -\frac{i}{2\hbar} \hat{p} \cdot \delta \hat{q}_{0}(t) \delta t \right] \exp \left( -\frac{1}{\hbar} m \hat{p} \cdot \delta \hat{q}_{0}(t) \right), \tag{C14}
\]

where \( \delta \hat{q}_{0}(t) \equiv \hat{q}_{0}(t + \delta t) - \hat{q}_{0}(t) \).

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