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I. INTRODUCTION

Studying the wave nature of localized single particles allows fundamental questions of quantum mechanics to be addressed. Recently, experimental progress has boosted this area and experiments that can control single particles have become available in various systems. These include neutral atoms in optical lattices [1–3] or microscopic dipole traps [4,5], electrons in quantum dots [6], and several other systems. One of the advantages of ultracold atomic systems is their purity and low-noise environment, which makes them well suited for applications in quantum metrology and information [7,8].

Developing a robust toolbox for engineering using the laws of quantum mechanics is therefore an important challenge. Compared to classical physics, many applications require coherent evolution not to be disturbed and one common process needed is a mechanism that allows transfer of particles between different trapping sites. Tunneling is such a mechanism; however, in its direct application it leads to Rabi oscillations, which make controlled experiments difficult [9]. Recently, a new method, termed coherent tunneling adiabatic passage (CTAP), has been suggested [10–13]; it is analogous to the three-level techniques of stimulated Raman adiabatic passage (STIRAP) in optical physics [14]. This technique allows for high-fidelity transport between different trapping sites, with adiabaticity as the only requirement. A first demonstration using optical waveguides was recently reported [15].

While STIRAP is a well-investigated technique in optical systems [14], which can be adapted for applications such as the creation of superposition states [16], its translation into the atom optical realm offers many new and interesting degrees of freedom to be explored. Recently, a number of studies have focused on the effects of nonlinear dynamics on the transfer process [13,17]. Here we add another degree of freedom by studying states with nontrivial phase distributions and show that the CTAP process is not robust with respect to conserving the phase and therefore the functional form of the density distribution. However, we also show that the process can still be used to control the phase of the quantum state in question. Phase engineering has become an important technique in the area of quantum computing recently and the convenience of adiabatic techniques is that if the associated energy eigenvalue is zero, one can make use of the usually much smaller geometrical phases [18–20]. While this is true for optical systems, we will show that one has to be more careful in atom-optical settings.

Tunneling of an individual vortex is an interesting problem in a number of systems, including Bose-Einstein condensates and Josephson junctions. The escape of a single vortex from a pinning potential in a Josephson junction has been investigated experimentally [21] and recently the tunneling of a vortex in a Bose-Einstein condensate has been the subject of a numerical study for double-well potentials [22]. Salgueiro et al. found that the topological defect is preserved on tunneling of the condensate and, in fact, can be replicated in such a way that each potential minimum has a single vortex [22].

In the following we will first give a brief introduction to the CTAP idea and show that the standard approximation of a three-level system is good for the density transport. We will then compare this approximation to the full integration of the Schrödinger equation for the problem and identify the problems for phase stability. Finally, we will extend the work to look at systems with small nonlinearities and conclude.

II. COHERENT TRANSPORT

The CTAP process for cold atoms considers a system of three microtraps, between which a single particle can tunnel (see Fig. 1). The strength of the tunneling is determined by the distance and barrier height between the individual traps. If one assumes all traps to be of the same shape (i.e., have resonant energy levels), and only allows for adiabatic processes, one can write the Hamiltonian in terms of the asymptotic eigenstates of the individual traps, $|L\rangle$, $|M\rangle$, and $|R\rangle$, as

$$H = \begin{pmatrix} 0 & J_{LM} & 0 \\ J_{LM} & 0 & J_{MR} \\ 0 & J_{MR} & 0 \end{pmatrix}.$$  (1)

The $J_{ij}$ are the tunneling matrix elements between neighboring traps and we assume the tunneling between nonneighboring traps to be negligible. The eigenstates and eigenvalues of this Hamiltonian are well known [14] and we will focus here on the so-called dark eigenstate given by

$$|D\rangle = \cos \theta |L\rangle + \sin \theta |R\rangle.$$  (2)
This state only has an indirect contribution from the central trap through the mixing angle, \( \tan \theta = J_{MR}/J_{LM} \), and its energy eigenvalue is given by \( E_D = 0 \). If one allows for time-dependent tunneling rates, this state can be used to transfer a particle from, say, trapping site |L\rangle to |R\rangle with large fidelity, even in the presence of noise [10–12]. Note that during this transfer the particle has no probability of ever being in the state |M\rangle.

To remind the reader, let us briefly review this transfer process: The tunneling frequencies can become functions of time through a time-dependent variation of the distance between the individual traps, through a modulation of the respective barrier heights, or through a combination of both of these. Here we will assume that the trap positions change in time and, since we will assume piecewise harmonic potentials, this will also lead to a decrease in barrier height. If we therefore first decrease the distance \( d_{MR} \), and, with a delay, the distance \( d_{LM} \), we create the familiar counterintuitive STIRAP timing sequence for the values of the tunneling strengths \( J_{MR} \) and \( J_{LM} \) [see Figs. 2(a) and 2(b) and calculations in the following]. During this process the mixing angle \( \theta \) changes from 0 to \( \pi/2 \) [see Fig. 2(c)], which allows a particle initially trapped on the left-hand side to be transferred to the trap on the right-hand side. This is the essence of the celebrated STIRAP technique.

To calculate the tunneling frequency between two traps as a function of trap distance, let us turn to the exactly solvable model system of piecewise harmonic traps [23,24], which also guarantees good approximate resonance between the levels at any point in time:

\[
V = \begin{cases} \frac{1}{2m} \omega^2 (x + \frac{d}{2})^2 & \text{for } x \leq 0, \\ \frac{1}{2m} \omega^2 (x - \frac{d}{2})^2 & \text{for } x \geq 0. \end{cases}
\]

The eigenfunctions of this potential are known to be given by parabolic cylinder functions [25]

\[
\psi_1(x) = N_1 D_v \left[ -\frac{2m\omega}{\hbar} \left( x + \frac{d}{2} \right) \right] \quad \text{for } x \leq 0, \quad \psi_2(x) = N_2 D_v \left[ \frac{2m\omega}{\hbar} \left( x - \frac{d}{2} \right) \right] \quad \text{for } x \geq 0,
\]

where \( N_1 \) and \( N_2 \) are the normalization constants. The eigenenergies are given by \( E/\hbar\omega = \nu + \frac{1}{2} \) and the quantum numbers, \( \nu \), are determined by requiring that the logarithmic derivatives of the two wave functions are equal at \( x = 0 \):

\[
\left( \frac{\psi_1'}{\psi_1} \right)_{x=0} = \left( \frac{\psi_2'}{\psi_2} \right)_{x=0}.
\]

By solving this condition we can exactly calculate the tunneling strength between the two traps at any time during the adiabatic process. If we then diagonalize Eq. (1) we find the eigenvalues displayed in Fig. 2(d), where the dark state with the eigenvalue of zero is clearly visible. Since we assume that the whole process is carried out adiabatically, the system will be in this state at any point in time.

### III. ANGULAR MOMENTUM STATE

In order to write down the Hamiltonian equation (1) for a realistic system a number of approximations must hold. First, the eigenstates of the isolated traps have to be in close resonance; second, the levels of the individual traps have to be chosen such that they are well isolated from all other available states in the system. The second condition can almost always be fulfilled by making the process more adiabatic and the first one translates into the simple requirement that all traps have the same trapping frequency (in case of harmonic traps). For realistic traps, however, this is problematic, as potential forces often add when they start to overlap. Several solutions have been proposed for this, including the use of time-dependent compensation potentials [12]. Here we assume that this is experimentally possible, as it allows us to isolate the physics relevant to the dynamics of the phase.

To examine the influence of the CTAP dynamics on the phase distribution of a quantum state let us first carry out a full numerical integration of the Schrödinger equation for a general system. This will at the same time function as a control mechanism for the approximations just made, in particular the fact that we neglected non-nearest-neighbor coupling and treated tunneling as a one-dimensional process. For numerical
simplicity, however, we will only consider a two-dimensional setup here, as this will allow us to capture the main physical processes. In scaled coordinates Schrödinger’s equation is therefore given by
\[
\frac{i}{\hbar} \frac{d}{dt} \psi(x,y) = \left( -\frac{1}{2} \nabla^2 + \frac{1}{2} V(x,y,t) \right) \psi(x,y),
\]
where \(V(x,y)\) is the trapping potential of the three traps in the linear configuration and which fulfills the conditions just outlined. For generality, all lengths are scaled with respect to the ground-state size of the individual harmonic traps, \(a_0 = \sqrt{\hbar/m\omega}\), where \(m\) is the mass of the particle and \(\omega\) the trapping frequency of the individual harmonic oscillator potentials. All energies are scaled in units of the harmonic oscillator energy, \(E_0 = \hbar\omega\), and time is in units of \(1/\omega\).

To be specific, let us choose an initial state that carries a single quantum of angular momentum and therefore has a phase distribution that increases by \(2\pi\) for a closed loop around the center of the state. This state is initially located in the trap on the left-hand side. We numerically integrate Eq. (7) where we have chosen \(d_{LM}^R\) and \(d_{MR}^L\) to follow sinusoidal paths [see Fig. 2(a)].

The results of the numerical integration are summarized in Fig. 3 and show surprising dynamics: While the process still leads to a 100% transfer of the probability amplitude to the trap on the right-hand side (not shown), the angular momentum of the final state oscillates continuously between clockwise and counterclockwise depending on the overall duration of the process (see upper part of the figure). Four examples of this change in phase and density associated with four different durations are shown in the lower half of the figure. In the first example (A) the system is in exactly the same state as it started, whereas in (B) the circulation of the flow has been reversed by the CTAP process. The plots (C) and (D) show the situation where the final state is in a superposition of clockwise and counterclockwise rotation, which also leads to a strongly modified density distribution.

This behavior might seem surprising at first, as angular momentum is usually thought of as a conserved quantity. However, in non-rotationally-symmetric geometries this conservation law does not hold and in fact can lead to interesting dynamics for vortices in anisotropic potentials [26–29]. As in our example the particle is tunneling between rotationally symmetric potentials, it is not \(a priori\) clear where the necessary asymmetry comes from.

To gain insight into this behavior, let us return to the three-state model and consider the transport of a particle in a harmonic oscillator potential carrying one unit of angular momentum. In two dimensions its energy is given by \(E_0 = 2\hbar\omega\) and the state is doubly degenerate, \(\psi_{n,n} = \psi_{10}\) and \(\psi_{n,n} = \psi_{01}\). We therefore have to write the most general wave function as the superposition
\[
\psi(x,y) = \psi_1(x)\psi_0(y) + i\psi_0(x)\psi_1(y)e^{-i\theta},
\]
where the one-dimensional, single-particle eigenfunctions of the harmonic oscillator for the ground and first excited state are given by \(\varphi_n\). We have also allowed for a relative phase \(\theta\) between the two degenerate states; however, we can set this initially to zero without loss of generality.

As our traps are arranged in a linear configuration along the \(y\) axis we can assume that the dynamics in the different spatial directions decouple. Tunneling therefore needs to be taken into account only for the wave function part in the \(y\) direction and we find that the Hamiltonian can be split into one for the ground-state parts of the wave function and one for the excited states,
\[
H_0 = \begin{pmatrix} \epsilon_0 & J_{LM} \cr J_{LM}^T & 0 \end{pmatrix} \begin{pmatrix} 0 & \epsilon_0 \cr \epsilon_0 & 0 \end{pmatrix} = \begin{pmatrix} J_{LM}^T & 0 \cr 0 & J_{LM} \end{pmatrix}
\]
and
\[
H_1 = \begin{pmatrix} \epsilon_1 & J_{LM} \cr J_{LM}^T & \epsilon_1 \end{pmatrix} \begin{pmatrix} 0 & \epsilon_0 \cr \epsilon_0 & 0 \end{pmatrix} = \begin{pmatrix} J_{LM}^T & 0 \cr 0 & J_{LM} \end{pmatrix}.
\]
Unlike in the previous section, we cannot simply set the diagonal elements equal to zero as now both the ground state and first excited energies are involved. However, each of the Hamiltonians still has a dark eigenstate with the eigenvalues \(\epsilon_0\) and \(\epsilon_1\), respectively. If initially a single particle is in the trap on the left-hand side in the state given by Eq. (8), after the CTAP process, these Hamiltonians lead to
\[
\begin{align*}
\psi_0^L(x) & \rightarrow \psi_0^L(x)e^{-i\epsilon_0 t_f}, \\
\psi_1^L(x) & \rightarrow \psi_1^L(x)e^{-i\epsilon_1 t_f}, \\
\psi_0^R(y) & \rightarrow \psi_0^R(y)e^{-i\epsilon_1 (t_f-\sqrt{x})}, \\
\psi_1^R(y) & \rightarrow \psi_1^R(y)e^{-i\epsilon_0 (t_f-\sqrt{x})},
\end{align*}
\]
where \(t_f\) is the overall duration of the process, \(\epsilon_{0y}, \epsilon_{1x}, \epsilon_{0x}, \) and \(\epsilon_{1y}\) are the ground and excited energies in the \(x\) and \(y\) directions, and the superscripts \(L\) (left) and \(R\) (right) refer to the traps in which the wave function is localized. One can immediately see that if \(\epsilon_{0y}\) and \(\epsilon_{1y}\) are not independent of time,
the wave function acquires a relative phase between the two degenerate states that is dependent on the overall duration of the CTAP process:

\[
\psi(x,y; t_f) = \psi_0^R(x)\psi_0^R(y)e^{-i[\epsilon_1, t_f + \int_{t_f}^0 \epsilon_0(t')dt']} + i\psi_0^R(x)\psi_1^R(y)e^{-i[\epsilon_0, t_f + \int_{t_f}^0 \epsilon_1(t')dt']},
\]

(15)

For easier understanding let us rewrite this state by defining a global and a relative phase as

\[
\gamma = \epsilon_1, t_f + \int_{0}^{t_f} \epsilon_0(t')dt',
\]

(16)

\[
\theta = -[\epsilon_1, - \epsilon_0]_{t_f} + \int_{0}^{t_f} [\epsilon_0(t') - \epsilon_1(t')]dt',
\]

(17)

so that we can write the final state as

\[
\psi(x,y; t_f) = e^{-i\gamma} \left[ \psi_0^R(x)\psi_0^R(y) + i\psi_0^R(x)\psi_1^R(y)e^{i\theta} \right].
\]

(18)

One can clearly see from this that any slight deviation in the difference between the asymptotic energy levels of the individual traps will have a significant effect on the final wave function. As, in particular, in realistic situations the shape of the individual potentials most likely strongly changes, one can expect to be unable to control the final form of the wave function. The CTAP process is therefore unstable with respect to states with nontrivial phase distributions [30]. However, as our example shows, this does not have to be a random process and in fact it can be used to engineer the phase of the wave function deterministically: By slightly changing the overall time of the process, one can cycle through all possible states for the fixed energy \( E_0 = 2\hbar \omega \).

Since in our simulations the potentials are piecewise harmonic, it is not immediately clear where the change in energies comes from. Let us therefore in the following carefully examine our model and determine the influence of various other degrees of freedom. The crucial point is that during the CTAP process the energy eigenstates in the \( y \) direction slightly change, since the potentials we are considering are only piecewise harmonic. By bringing them closer together, the height of the barrier between them changes, leading to a different asymptotic eigenstate. In fact, the eigenstates are very close to the parabolic cylinder functions defined earlier. As the first excited eigenstate is closer to the local maximum separating the traps, it will be shifted differently compared to the ground state. While the difference might only be small, the integration over a long, adiabatic time interval will lead to a large value for the integral. To demonstrate this, we show in Fig. 4 the energies for an atom in the state \( \phi_0(y) \) and \( \phi_1(y) \), \( \epsilon_{0y} \) and \( \epsilon_{1y} \), respectively, during the CTAP process. It can be clearly seen that at the time of approach the energy eigenvalues slightly change, as previously assumed. In addition, we show that their difference, which is the integrand of Eq. (17), is not constant and thus gives rise to the time-dependent \( \theta(t_f) \).

From this argument it follows that the effect should depend not only on the overall time of the process but also on the minimum distance to which the traps approach each other. In Fig. 5, we show the resulting oscillations of angular momentum for a number of different values for \( d_{min} \). As the minimum distance is increased, the period of the oscillations increases as well (see the inset of Fig. 5), which is in accordance with the explanation just given: A larger minimum distance between the traps means that the energy levels are deviating less from the asymptotic values for perfect harmonic potentials. Let us also note that the observed behavior can also be interpreted as a variant of Ramsey interferometry, where the energy difference between the eigenenergies into two different spatial directions leads to a phase difference.

IV. NONLINEAR CTAP

Let us finally discuss the effect of a nonlinearity on the evolution of the phase. The paradigm of an atomic nonlinear system of well-defined phase is a Bose-Einstein condensate and its dynamics can be described by the so-called Gross-Pitaevskii equation

\[
\frac{i}{\hbar} \frac{d}{dt} \psi(x,y) = \left( -\frac{1}{2} \nabla^2 + V(x,y) + \frac{U}{2} |\psi|^2 \right) \psi(x,y).
\]

(19)

FIG. 4. (Color online) Evolution of \( \epsilon_{0y} \) (blue dashed), \( \epsilon_{1y} \) (green dot-dashed), and \( \epsilon_{0y} - \epsilon_{1y} \) (red solid) over the course of the CTAP process. Both energies are initially separated by \( \omega = 1 \), but they do not maintain this separation due to the modification of the potential as the traps move closer together. Time is measured in units of \( 1/\omega \) and energy in units of \( \hbar \omega \).

FIG. 5. (Color online) Final angular momentum as a function of time for different minimum distances between the traps: \( d_{min} = 2.0 \) (full line), \( d_{min} = 2.2 \) (dashed line), and \( d_{min} = 2.4 \) (dotted line). The offset of the different curves has been shifted for clarity. The inset shows the increase of the period with increasing \( d_{min} \). Time is measured in units of \( 1/\omega \) and angular momentum in units of \( \hbar \).
states in Bose-Einstein condensates in a controlled way, as
not shown). We therefore speculate that the effect described
only effects are an offset and a small reduction in periodicity
is that the oscillatory behavior of the angular momentum does
nonlinearity has on the final phase. The first thing to notice
will restrict ourselves to only small nonlinearities (µ ≪ ℏω),
for which about 100% transfer can still be reached.

In Fig. 6 we show the effect a small but increasing
nonlinearity has on the final phase. The first thing to notice
is that the oscillatory behavior of the angular momentum does
not get immediately suppressed by the nonlinearity and that
the only effects are an offset and a small reduction in periodicity
(not shown). We therefore speculate that the effect described
in this work can also be used to create vortex superposition
states in Bose-Einstein condensates in a controlled way, as
long as the samples are only weakly interacting. As it is well
known that vortex oscillations in an anisotropic potential can
be suppressed for large enough nonlinearities [26,28], it might
be interesting to study this effect in the presence of resonance
restoring techniques.

V. CONCLUSION

We have shown that the spatial CTAP process for atoms
in microtraps does not conserve the wave function form
for states with nontrivial phase distribution. This is due to
an unavoidable small time dependence of the asymptotic
eigenstates of the individual traps in the different spatial
directions, which results from the trap overlap. While each
experimental system will have its own specific dependence,
the instability is fundamentally present.

At the same time we have shown that this instability behaves
deterministically with respect to a change in the overall time
of the CTAP process and can therefore be used to create
well-defined angular momentum superposition states. Such
states can have applications in quantum information and have
recently seen a surge in interest [34,35]. We have also shown
that the presented process even survives in the presence of
small nonlinearities, therefore allowing the superposition of
vortices in Bose-Einstein condensates.

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[24] Note that an approximate formula for the tunneling strength between two harmonic traps of the same frequency $\omega$ at a distance $d$ was given in [10] as

$$J(d) = \frac{e^{d^2} (1 + d [1 - \text{erf}(d)]) - 1}{\sqrt{\pi} (e^{2d^2} - 1)/2d}.$$ 


[30] Note that in one dimension this process would only lead to a global phase and therefore states with nontrivial phase distributions (e.g., dark solitons) would not be affected.


