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<tr>
<td>Publication date</td>
<td>2015</td>
</tr>
<tr>
<td>Type of publication</td>
<td>Article (peer-reviewed)</td>
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</table>
[http://dx.doi.org/10.1103/PhysRevA.92.043406](http://dx.doi.org/10.1103/PhysRevA.92.043406)  
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Fast quasiadiabatic dynamics

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(Received 20 November 2014; published 7 October 2015)

We work out the theory and applications of a fast quasiadiabatic approach to speed up slow adiabatic manipulations of quantum systems by driving a control parameter as near to the adiabatic limit as possible over the entire protocol duration. We find characteristic time scales, such as the minimal time to achieve fidelity 1, and the optimality of the approach within the iterative superadiabatic sequence. Specifically, we show that the population inversion in a two-level system, the splitting and cotunneling of two-interacting bosons, and the stirring of a Tonks-Girardeau gas on a ring to achieve mesoscopic superpositions of many-body rotating and nonrotating states can be significantly speeded up.

DOI: 10.1103/PhysRevA.92.043406 PACS number(s): 32.80.Xx, 67.85.—d, 03.75.Kk

I. INTRODUCTION

Developing technologies based on delicate quantum coherences of atomic systems is a major scientific and technical challenge due to pervasive noise-induced and manipulation errors. Shortening the process below characteristic decoherence times provides a way out to avoid the effects of noise, but the protocol (time dependence of control parameters) should still be robust with respect to offsets of the external driving parameters. Shortcuts to adiabaticity (STA) are a set of techniques to reduce the duration of slow adiabatic processes, minimizing noise effects while keeping or enhancing robustness [1–3]. There are different approaches but they are not always easy to implement in practice, because of the need to control many variables, or the difficulty to realize certain terms added to the original Hamiltonian to speed up the adiabatic dynamics. Here we work out the theory and present several applications of a simple, but effective, fast quasiadiabatic (FAQUAD) approach that engineers the time dependence of a single control parameter λ(t), without changing the structure of the original Hamiltonian, $H[\lambda(t)]$, to perform a process as quickly as possible while making it as adiabatic as possible at all times. The two goals are contradictory so a compromise is needed. We impose that the standard adiabaticity parameter $|\lambda(t)|$ is constant throughout the process, and consistent with the boundary conditions (BC) of $\lambda(t)$ at $t = 0$ and $t = t_f$.

In the simplest scenario we assume that the adiabatic process driven by changing $\lambda(t)$ involves a passage through at least one avoided crossing. While real systems are in general multilevel, only the two quasicrossing levels (say $E_1$ and $E_2$) in the instantaneous basis $|\phi_i\rangle$ need to be considered under the adiabaticity condition [4], $|\langle \phi_1(t)|\partial_\lambda \phi_2(t)\rangle_{E_1(t) - E_2(t)}| \ll 1$. (More levels can be taken into account if necessary.) Then impose

$$h |\langle \phi_1(t)|\partial_\lambda \phi_2(t)\rangle_{E_1(t) - E_2(t)}| = h |\langle \phi_1(t)|\frac{\partial E(t)}{\partial \lambda} \phi_2(t)\rangle_{E_1(t) - E_2(t)}| = c,$$  

and as $\lambda(t) = \lambda(t)$ and $t = t(\lambda)$ we apply the chain rule to write

$$\dot{\lambda} = \mp \frac{c}{h} \frac{E_1(\lambda) - E_2(\lambda)}{|\langle \phi_1(\lambda)|\partial_\lambda \phi_2(\lambda)\rangle|^2} = \mp \frac{c}{h} \frac{[E_1(\lambda) - E_2(\lambda)]^2}{|\langle \phi_1(\lambda)|\partial_\lambda \phi_2(\lambda)\rangle|^2}.$$  

where the overdot is a time derivative and $\mp$ applies to a monotonous decrease or increase of $\lambda(t)$. Equation (2) must be solved with the BC $\lambda(0)$ and $\lambda(t_f)$, which fixes $c$ and the integration constant. The corresponding FAQUAD solution, $\lambda_F(t)$, changes quickly when the transitions among instantaneous eigenstates are unlikely and slowly otherwise. An equation equivalent to Eq. (2) has been applied to specific models [5–10], for example, the two-level system [7] and three-level lambda systems [6].

In this paper, we derive important properties of FAQUAD including characteristic time scales, such as the minimal time to achieve fidelity 1, and its optimality within the iterative superadiabatic sequence. We also apply FAQUAD to several physical systems for which other shortcut techniques are difficult or impossible to implement, including a process for creating a collective superposition state between rotating and nonrotating atoms on a ring.

The FAQUAD strategy belongs to a family of processes that use the time dependence of a control parameter to delocalize in time the transition probability among adiabatic levels. In the parallel adiabatic transfer technique [11,12] the level gap is required to be constant, which prevents it from being applicable when the initial and final gaps are different [see the Tonks-Girardeau (TG) gas example below]. The uniform adiabatic (UA) method developed in [13] relies on a comparison of transition and relaxation time scales and predicts (in a notation consistent with the one used in the work) $\dot{\lambda} = \mp c_{LA} \frac{|E_1(\lambda) - E_2(\lambda)|^{3/2}}{|\langle \phi_1(\lambda)|\partial_\lambda \phi_2(\lambda)\rangle|^2}$. Furthermore, the local adiabaticity (LA) approach [14,15] predicts an equation similar to Eq. (2), however without the factor $|\langle \phi_1(\lambda)|\partial_\lambda \phi_2(\lambda)\rangle|^2$. This leads to a different constant, $c_{LA}$, and time dependence of the parameter, $\lambda_{LA}(t)$, and therefore different minimal times as illustrated below. Note that in [14] Eq. (2) is also written down but not applied as such.

II. GENERAL PROPERTIES

We rewrite Eq. (2) in terms of $s = t/t_f$ and define $\tilde{\lambda}(s) := \lambda(st_f)$ so that $\lambda(t) = \tilde{\lambda}(\frac{t}{t_f})$, where the prime is the derivative.

1050-2947/2015/92(4)/043406(6) 043406-1 ©2015 American Physical Society
with respect to $s$. We get
\[ \tilde{\lambda}' = \frac{\hbar}{E_1 - E_2} \left| \langle \phi_1 | \partial_s \phi_2 \rangle \right|, \tag{3} \]
with
\[ \tilde{c} = ct_f = \pm \hbar \int_{\tilde{\lambda}(0)}^{\tilde{\lambda}(1)} \frac{d\tilde{\lambda}}{E_1 - E_2 \langle \phi_1 | \partial_s \phi_2 \rangle}. \tag{4} \]

It is thus enough to solve the FAQUAD protocol once, i.e., using Eq. (3) we get $\tilde{\lambda}_f(s)$ and $\tilde{c}$ to satisfy $\tilde{\lambda}(s = 0)$ and $\tilde{\lambda}(s = 1)$, and then adapt (scale) the result for each $t_f$, as $\lambda_f(t = st_f) = \tilde{\lambda}_f(s)$, and $c = \tilde{c}/t_f$. Similarly, the gap $\omega_{12}(t) = |E_1(t) - E_2(t)|/\hbar$ is given in terms of a universal gap function $\omega_{12}[\lambda_f(s)]$ as $\omega_{12}(t) = \omega_{12}[\lambda_f(t/t_f)]$. Depending on $\tilde{c}$, a large time $t_f$ might be necessary to make the process fully adiabatic (i.e., with a small enough $c$) but, surprisingly, much shorter times for which the process is not fully adiabatic also lead to the desired results. Since the system is nearly adiabatic this is explained by adiabatic perturbation theory. In the adiabatic basis the wave function is expanded as $|\Psi(t)\rangle = \sum_n g_n(t)e^{i\phi_n(t)}|\phi_n\rangle$, where $g_n(t) = -i \int_0^t E_n(t')dt' + i \int_0^t \langle \phi_n(t') | \partial_s \phi_n(t') \rangle dt'$. From $i\hbar|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$ we get, choosing $\langle \phi_n(t') | \phi_n(t') \rangle$ to be real (in particular $\langle \phi_n(t') | \phi_n(t) \rangle = 0$),
\[ \dot{g}_n = -\sum_{k \neq n} e^{iW_{nk}(t') \langle \phi_n(t') | \frac{\partial}{\phi_k(t')} \rangle} g_k(t), \tag{5} \]
where $W_{nk}(t) = \int_0^t \omega_{nk}(t')dt'$ is a dynamical-gap phase and $\omega_{nk}(t) := [E_n(t) - E_k(t)]/\hbar$. Integrating,
\[ g_n(t) - g_n(0) = -\sum_{k \neq n} \int_0^t e^{iW_{nk}(t') \langle \phi_n(t') | \phi_k(t') \rangle} \dot{g}_k(t')dt', \tag{6} \]
which is still exact. Assuming that the initial state is $|\phi_m(0)\rangle$ and approximating $g_n(t') = \delta_{nm}$ one finds to first order, for $n \neq m$,
\[ g_n^{(1)}(t) = -\int_0^t \langle \phi_n(t') | \frac{\partial}{\phi_m(t')} \rangle e^{iW_{nm}(t')}dt', \tag{7} \]
which should satisfy $|g_n(t)| \ll 1$ for an adiabatic evolution. In FAQUAD, setting $n = 2$ and $m = 1$ and neglecting transitions to further states, $\langle \phi_2(t') | \phi_1(t) \rangle = r \omega_{21}(t)$, with $r = \text{sgn}(\langle \phi_2(t') | \phi_1(t) \omega_{21} \rangle)$, so we find (higher-order corrections are also explicit)
\[ g_2^{(1)}(t) = -r \int_0^t \omega_{21}(t')e^{iW_{21}(t')}dt' = -icr e^{iW_{21}(t) - 1}. \tag{8} \]

Note the scaling $W_{21}(t_f) = t_f\Phi_{11}$ where $\Phi_{11} = \int_0^t \omega_{21}(s)ds$, and $\omega_{21}(s) = \omega_{21}(st_f)$. The oscillation period for the final population with FAQUAD is $T = \frac{2\pi}{2\Phi_{11}}$, which is also a good estimate of the minimal (final) time to pass through the avoided crossing with fidelity 1 [since $g_2^{(1)}(T) = 0$]. The upper envelope for the probability of level 2 is $4e^{2}/t_f^2$. The period, envelope, and Eq. (8) are important general results of this work. The oscillation is due to a quantum interference: $g_2^{(1)}(t_f)$ results from the sum of paths where the jump at time $t'$ from 1 to 2 has an amplitude $\omega_{21}(t')$. $e^{iW_{21}(t')}$ represents the dynamical phases before and after the jump, as $e^{iW_{21}(t')} = e^{\frac{2\pi}{\Phi_{11}} t'} dt'E_2(t')e^{\frac{2\pi}{\Phi_{11}} t'} dt'E_2(t')e^{\frac{2\pi}{\Phi_{11}} t'} dt'E_2(t')$, where the last exponential is a phase factor independent of $t'$.

To illustrate these general properties, we will first examine the two-level model, a paradigmatic test bed. Then, to show the power of FAQUAD, we will apply it to more complicated atomic systems.

### III. POPULATION INVERSION

Consider first a two-mode model with a single avoided crossing. In the bare basis, $|1\rangle = |\phi_1\rangle$ and $|2\rangle = |\phi_2\rangle$, the time-dependent state is $|\Psi(t)\rangle = b_1(t)|1\rangle + b_2(t)|2\rangle$ and
\[ H = \begin{pmatrix} 0 & -\sqrt{2}J \\ -\sqrt{2}J & U - \Delta \end{pmatrix}, \tag{9} \]
where the bias $\Delta = \Delta(t)$ is the control parameter, and $U > 0$ and $J > 0$ are constant. The instantaneous eigenvalues are
\[ E_1 = \frac{1}{2}(U - \Delta - P), \tag{10} \]
\[ E_2 = \frac{1}{2}(U - \Delta + P), \tag{11} \]
where $P = P(t) = \sqrt{8}J^2 + U^2 - 2U\Delta(t) + \Delta^2(t)$, and the normalized eigenstates are
\[ |\phi_1\rangle = \frac{1}{\sqrt{1 + (U - \Delta + P^2)/8J^2}} \left( \frac{1}{\sqrt{2}}(U - \Delta + P) \right) |1\rangle \tag{12} \]
\[ |\phi_2\rangle = \frac{1}{\sqrt{1 + (U - \Delta + P^2)/8J^2}} \left( \frac{1}{\sqrt{2}}(U - \Delta - P) \right) |2\rangle. \tag{13} \]

The goal is to drive the eigenstate from $|\phi_1(0)\rangle = |2\rangle$ to $|\phi_2(t_f)\rangle = |1\rangle$. To design the reference adiabatic protocol we impose on $\Delta(t)$ the BC $\Delta(0) \gg U, J$ and $\Delta(t_f) = 0$. The FAQUAD protocol is shown in Fig. 1(a) compared to a linear-in-time $\Delta(t)$ and a constant $\Delta = U$. The final ground-state populations $|b_1(t_f)|^2$ versus dimensionless final time $\tau_f = Jt_f/\hbar$ are shown in Fig. 1(b). Since the dressed states are essentially pure bare states at initial and final times their populations in bare and dressed state bases coincide at these times. For $\Delta = U$ between $t = 0$ and $t_f$, “Rabi oscillations” (we use a terminology appropriate for quantum optics but of course the two-level model is more broadly applicable) occur [see Fig. 1(b)]. The conditions for a $\pi$ pulse or multiple $\pi$ pulses are met periodically over $t_f$ alternated with times where the probability drops to zero because of destructive interference among two dressed states superposed with equal weights. By contrast the FAQUAD process is dominated by one dressed state and the influence of the transitions to the other one is minimized, because they are small in amplitude, and because at certain times they completely cancel each other out by destructive interference. The time interval between population maxima for FAQUAD is $2\pi/\Phi_{1,2}$ [also shown in Figs. 1(b) and 1(d) by stars], i.e., it is not governed by the Rabi frequency. The first maximum is at a small $t_f$ similar to the one for the $\pi$ pulse, but broader. The FAQUAD maxima are more stable with respect to errors in $\Delta$ as $t_f$ increases, whereas
the flat-pulse maxima decrease their stability. Figure 1(b) also shows the poorer results of the linear ramp for $\Delta(t)$.

FAQUAD is compared to the LA and UA approaches in Figs. 1(c) and 1(d). It provides shortcuts at smaller process times (it achieves 0.9998 probability three times faster than LA) and an analytically predictable behavior via the perturbation theory analysis. Let us now consider more complicated atomic systems where FAQUAD can be applied whereas other STA techniques cannot.

IV. INTERACTING BOSONS IN A DOUBLE WELL

Pairs of interacting bosons in a double-well potential may be manipulated to implement universal quantum logic gates for quantum computation or to observe fundamental phenomena such as cotunneling of two atoms [17,18]. We shall speed up two processes: the splitting of the two particles from one to the two separate wells, and cotunneling (see Fig. 2). The boson dynamics in a double well with tight lateral confinement is described by a two-site Bose-Hubbard Hamiltonian [17]. The Hamiltonian in the occupation number basis $|2,0\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, $|0,2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is

$$H = \begin{pmatrix} U + \Delta & -\sqrt{2}J & 0 \\ -\sqrt{2}J & -\sqrt{2}J & U - \Delta \\ 0 & -\sqrt{2}J & U + \Delta \end{pmatrix}, \quad (14)$$

where the bias $\Delta = \Delta(t)$ is the control function, $J$ is the hopping energy, and $U$ is the interaction energy. We write the time-dependent states as $|\Psi(t)\rangle = c_1(t)|2,0\rangle + c_2(t)|1,1\rangle + c_3(t)|0,2\rangle$. Adiabatic processes that change $\Delta(t)$ slowly, keeping the $U/J$ ratio constant, are possible to implement splitting or cotunneling. Speeding them up by a “counterdiabatic” approach is not possible in practice because of the need to apply new terms in the Hamiltonian which are difficult to implement. Alternative techniques could not be applied [19] or are cumbersome [20,21] because of the relatively large algebra involved. The FAQUAD approach provides a viable way out.

In a splitting process $\Delta(0) \gg U/J$ and $\Delta(t_f) = 0$ [see Fig. 2(a)]. The initial ground state is $|\phi_i\rangle = |0,2\rangle$ and the final ground state $|\phi_f\rangle = |1,1\rangle$. Figure 3(a) shows the dependence of the three eigenenergies with $\Delta$. $\Delta(t)$ is very similar to the result for the two-level system in Fig 1(a). The results of FAQUAD and the linear protocol are compared in Fig. 3(b). The probability of the first peak for FAQUAD, 0.998 at $t_f = 1.2$, is achieved with the linear ramp for $t_f = 43$.

In a speeded-up cotunneling shown in Fig. 2(b) the goal is to drive the system fast from $|\phi_i(0)\rangle = |0,2\rangle$ to $|\phi_f(t_f)\rangle = |2,0\rangle$ intermediated by $|1,1\rangle$ [the Hamiltonian (14) does not connect $|2,0\rangle$ and $|0,2\rangle$ directly]. We impose $\Delta(0) \gg U/J$ and $\Delta(t_f) = -\Delta(0)$ to have $|0,2\rangle$ and $|2,0\rangle$ as the ground state at initial and final times, respectively. The energy levels versus $\Delta$ are depicted in Fig. 3(a) for repulsive interaction ($U > 0$). Figure 4(a) shows the FAQUAD trajectory for $\Delta(t)$ for the repulsive strong-interaction regime, $U/J = 22.3$. Figure 4(b) depicts the final probabilities of the bare state $|2,0\rangle$ for FAQUAD and a linear protocol that needs about $t_f = 65$ to achieve the value of the first peak of the FAQUAD method ($|c_1|^2 = 0.998$ at $t_f = 2.3$). The minima in the FAQUAD probability go in this case below the lower envelope $1 - 4|c_2|^2/t_f^2$ predicted by perturbation theory. The reason is a leak through the narrow avoided crossing at $\Delta = 0$ from the second to the third energy level [see Fig. 3(a)]. The leak occurs at total
V. COLLECTIVE SUPERPOSITIONS OF ROTATING AND NONROTATING ATOMS ON A RING

Creating a macroscopic or mesoscopic superposition of a many-particle system is a difficult task and of interest for research in quantum information, quantum metrology, and fundamental aspects of quantum mechanics. However, it was recently proposed that a low-dimensional gas of interacting bosons in the TG limit [22] placed on a ring can be perturbed in such a way that a robust superposition of two angular momentum states can be achieved. This perturbation corresponds to the introduction of a narrow potential, which is then accelerated to a certain value to spin up the gas [23].

For a single particle this is described by

\[
i \hbar \partial_t \psi(x,t) = \left\{ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + U_0 \delta[x - x_0(t)] \right\} \psi(x,t),
\]

where the stirrer is represented by a \( \delta \) function of strength \( U_0 \) and periodic BC are assumed. In a comoving frame one can then define \( y = x - x_0(t) \) and the Hamiltonian is \( H = \frac{1}{2M} (\hat{P}_y - \hbar \Omega(t)/L)^2 + U_0 \delta(y) \), where \( L \) is the ring perimeter, \( \hbar \Omega(t) \equiv \hbar \omega_n(t) \), and \( \hat{P}_y \equiv -i \hbar \partial / \partial y \). The instantaneous energy eigenvalues are \( E_n = \frac{n^2 \hbar^2 \omega_n^2}{2M} \) and the \( \omega_n \) are solutions of

\[
4\pi \hbar^2 \omega_n = \cos(n \pi \alpha_n - \Omega / 2) + \cos(n \pi \alpha_n + \Omega / 2).
\]

For \( U_0 \to 0 \), the \( \omega_n \) tend to \( n - \Omega/(2\pi) \), with \( n = 0, \pm 1, \pm 2, \ldots \), where the different signs are for clockwise or counterclockwise rotation in the laboratory frame, and the \( n \)th eigenstates are plane waves with momentum \( n\hbar 2\pi / L \). For \( 0 < \Omega \ll \hbar \) the energies in the moving frame increase for \( n \leq 0 \) and decrease for \( n > 0 \). For \( U_0 = 0 \) the spectrum shows degeneracies at \( \Omega = 0, \pm \pi \), which turn into avoided crossings once the stirrer couples different angular momentum eigenstates, as shown in Fig. 5(a). Adiabatically increasing the stirring frequency from \( \Omega = 0 \) to \( \pi \) then allows us to drive the system into a superposition of two angular momentum states and for a TG gas with an odd number of particles \( N \) it can be shown that the ground state at \( \Omega = \pi \) corresponds to macroscopic superposition between states with angular momentum zero and \( N \hbar \).

To design an optimal \( \Omega(t) \) for the TG gas, we note that the fidelity depends mostly on leakage from the highest occupied levels. This can be seen by considering the time evolved TG gas state \( \Psi_{TG}(x_1, x_2, \ldots , x_N) \) defined by

\[
\Psi_{TG} = \frac{1}{\sqrt{N!}} \prod_{i<j} \text{sgn}(x_i - x_j) \sum_{\mu \in P} \epsilon_{\mu} \psi_{\mu_1}(x_1) \cdots \psi_{\mu_N}(x_N),
\]

where \( P \) represents the set of all permutations of \( \{0,1, \ldots , N-1\} \), \( \epsilon_{\mu} \) is the antisymmetric tensor of the permutation \( \mu \), and \( \psi_i \) are the one-particle orbitals. Assuming that the system is isolated and contains only \( N \) eigenvectors \( \phi_\mu \), the orbitals can be expressed as \( \psi_i = \sum_j U_{ij} \phi_j \) with \( U \) some unitary operator. If we now compare \( \Psi_{TG} \) to the ground state \( \Phi_{TG} \) of the TG gas at the final \( \Omega \), we can calculate the fidelity \( F = |\langle \Phi_{TG} | \Psi_{TG} \rangle| \) as

\[
F = \frac{1}{N!} \sum_{\nu,\mu} \epsilon_{\nu} \epsilon_{\mu} |\langle \phi_{\nu_1} | \psi_{\mu_1} \rangle \cdots \langle \phi_{\nu_N} | \psi_{\mu_N} \rangle| = \frac{1}{N!} \sum_{\nu,\mu} \epsilon_{\nu} \epsilon_{\mu} |U_{\mu_1,\nu_1} \cdots U_{\mu_N,\nu_N}| = |\text{det}(U)| = 1,
\]

since \( U \) is unitary. Of course, in reality the system we consider contains more than \( N \) eigenvectors and the fidelity does not remain 1, but this argument shows that leaking between two occupied states does not influence the fidelity of a TG gas at all; only leaks into modes above the Fermi level do, such as with nonzero mixing terms \( U_{N,N+1} \). We should therefore optimize \( \Omega_f(s) \) for the avoided crossing of the highest occupied level as shown in Fig. 5(b). The corresponding final-state fidelities for \( N = 3 \) and 9 with respect to the exact ground states clearly outperform the ones for the linear ramp [see Fig. 6(a)]. The linear ramp fidelity deteriorates as \( N \) increases whereas, remarkably, the fidelity of the FAQQUAD protocol stays constant. The effect of an error of the form \( \Delta \Omega(t) = \Omega_f(t)(1 + \epsilon) \) is shown in Fig. 6(b).

VI. DISCUSSION

The FAQQUAD approach to speed up adiabatic manipulations of quantum systems achieves significant time shortening by distributing homogeneously the adiabaticity parameter along the process while satisfying the boundary conditions of the control parameter. We have derived general time scales and we have demonstrated its applicability in different systems.
FIG. 6. (Color online) (a) Fidelity \(|\langle \Psi_{TD}(t) | \Phi_{TD} \rangle| \) for \( N = 3 \) [FAQUAD (solid black line) and linear \( \Omega(t) \) (short-dashed red line)] and \( N = 9 \) [FAQUAD (blue circles) and linear \( \Omega(t) \) (green triangles)]. \( \Psi_{TD}(t) \) is the time-evolved TG state starting from the ground state for \( \Omega = 0 \), and \( \Phi_{TD} \) is the ground state of the TG gas at \( \Omega = \pi \). (b) Fidelity \(|\langle \Psi_{TD}(t) | \Phi_{TD} \rangle| \) vs \( \epsilon \) if FAQUAD is applied following a wrong \( \Omega(t) = \Omega_{g}(t)(1 + \epsilon) \) for \( N = 3 \) (solid black line) and \( N = 9 \) (short-dashed red line). Here \( U_0 M L / \hbar^2 = 0.5 \).

in particular where other approaches are not available, and expect a broad range of applications, in quantum, optical, and mechanical systems, due to the ubiquity of adiabatic methods.

A natural extension is to attempt a scheme similar to Eq. (1) in a superadiabatic rather than an adiabatic frame [24]. A brief summary is provided here. Let us start with a Schrödinger picture Hamiltonian \( H_0(t) \) and corresponding wave function \( \psi_0(t) \). Defining the unitary operator \( A_0(t) = \sum_n | \phi_n(t) \rangle | n \rangle \) with \( | \phi_n(t) \rangle \) the adiabatic basis in Eqs. (12) and (13) and \( | n \rangle \) the bare basis, the Hamiltonian that governs the dynamics of the interaction picture state \( A_0^\dagger \psi_0 \)

\[
H_I(t) = \frac{1}{2} \sum_{\{U, J, \Omega\}} i \sqrt{2J} \hbar \Delta \left( \frac{U - P - \Delta}{\hbar} \right),
\]

with instantaneous eigenvalues

\[
E_{1}^{(1)} = \frac{1}{2} \left( U - \Delta + \sqrt{P^6 + 8 J^2 \hbar^2 \Delta^2} \right),
\]

\[
E_{2}^{(1)} = \frac{1}{2} \left( U - \Delta + \sqrt{P^6 + 8 J^2 \hbar^2 \Delta^2} \right),
\]

and normalized eigenstates

\[
| \phi_1^{(1)} \rangle = \left( \frac{2 \sqrt{2 J} \hbar \Delta}{(P^6 + 8 J^2 \hbar^2 \Delta^2)^{1/4}} \left( \sqrt{P^6 + \sqrt{P^6 + 8 J^2 \hbar^2 \Delta^2}} \right)^{1/4} \right),
\]

\[
| \phi_2^{(1)} \rangle = \left( \frac{2 \sqrt{2 J} \hbar \Delta}{(P^6 + 8 J^2 \hbar^2 \Delta^2)^{1/4}} \left( \sqrt{P^6 + \sqrt{P^6 + 8 J^2 \hbar^2 \Delta^2}} \right)^{1/4} \right).
\]

The first superadiabatic frame is defined by the unitary operator

\[
A_1(t) = \sum_n | \phi_n^{(1)} \rangle | n \rangle .
\]

The state \( A_1^\dagger \psi_1 \) is governed by the Hamiltonian

\[
H_1(t) = A_1^\dagger (H_1 - K_1) A_1,
\]

where \( K_1 = i \hbar A_1^\dagger A_1 \).

Note that superadiabaticity, i.e., the possibility to neglect \( K_1 \), does not necessarily imply adiabaticity, which amounts to neglecting \( K_0 \). Also, a shortcut to superadiabaticity is only a STA if the superadiabatic states \( | \phi_n^{(1)} \rangle \) coincide, up to phase factors, with the eigenstates of \( H_0 \), \( | \phi_0 \rangle \), at boundary times. This will imply additional boundary conditions on the control parameter. The equation that substitutes Eq. (1) for the lowest superadiabatic scheme beyond the adiabatic level is

\[
\dot{\phi}_1^{(1)}(t) = \frac{\hbar}{E_1^{(1)} - E_2^{(1)}} \left( \phi_1^{(1)}(t) \right),
\]

Using Eqs. (21)–(24) in Eq. (26), we get a second-order differential equation for \( \Delta \):

\[
\frac{\sqrt{J} \hbar}{(P^6 + 8 J^2 \hbar^2 \Delta^2)^{3/2}} = c.
\]

To satisfy \( | \phi_1^{(1)}(0) \rangle = | \phi_1(0) \rangle = | 2 \rangle \) and \( | \phi_1^{(1)}(t_f) \rangle = | \phi_1(t_f) \rangle = | 1 \rangle \) (up to phase factors) we have to impose four boundary conditions,

\[
\Delta(0) \gg U, J, \Delta(t_f) = 0,
\]

\[
\Delta(0) = 0, \Delta(t_f) \gg \Delta(0), U, J,
\]

that cannot be satisfied with two integration constants plus the \( c \). The mismatch between number of conditions and free parameters actually gets worse when increasing the order of superadiabaticity in further iterations. In the second superadiabatic frame defined by the unitary operator \( A_2(t) = \sum_{\{U, J, \Omega\}} | \phi_n^{(2)} \rangle | n \rangle \), due to the \( K_2 = i \hbar A_2^\dagger A_2 \) term, second-order derivatives of the control parameter appear in the superadiabatic eigenstates, so the number of boundary conditions necessary to satisfy \( | \phi_1^{(2)}(0) \rangle = | \phi_1(0) \rangle = | 2 \rangle \) and \( | \phi_1^{(2)}(t_f) \rangle = | \phi_1(t_f) \rangle = | 1 \rangle \) (up to phase factors) increases to 6. Moreover, the differential equation resulting from applying the FAQUAD concept in the second superadiabatic basis is of third order in \( \Delta \). Once again, the differential equation cannot satisfy the six boundary conditions with three integration constants plus the \( c \). In general, as the order of the iteration increases, the number of boundary conditions to satisfy grows as \( 2n + 2 \), where \( n \) is the order of the iteration, while the order of the differential equation increases as \( n + 1 \). Hence, the adiabatic frame is in fact optimal to apply the FAQUAD concept within the series of iterative superadiabatic frames, as it is the only one for which the number of conditions equals the number of free parameters available.

**ACKNOWLEDGMENTS**

We thank M. Palmero, D. Guéry-Odelin, X. Chen, and S. Ibáñez for discussions. Support by the Basque Country Government (Grant No. IT472-10), Ministerio de Economía y Competitividad (Grant No. FIS2012-36673-C03-01), program UFI 11/55 of UPV/EHU, and the Okinawa Institute of Science.
and Technology Graduate University is acknowledged. This publication has emanated from research conducted with the financial support of Science Foundation Ireland under the International Strategic Cooperation Award Grant No. SFI/13/ISCA/2845. S.M.-G. acknowledges a fellowship by UPV/EHU.