Robust state preparation in quantum simulations of Dirac dynamics

Xue-Ke Song,1,2 Fu-Guo Deng,2 Lucas Lamata,1 and J. G. Muga1

1Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain
2Department of Physics, Applied Optics Beijing Area Major Laboratory, Beijing Normal University, Beijing 100875, China

(Dated: November 26, 2018)

A non-relativistic system such as an ultracold trapped ion may perform a quantum simulation of a Dirac equation dynamics under specific conditions. The resulting Hamiltonian and dynamics are highly controllable, but the coupling between momentum and internal levels poses some difficulties to manipulate the internal states accurately in wave packets. We use invariants of motion to inverse engineer robust population inversion processes with a homogeneous, time-dependent simulated electric field. This exemplifies the usefulness of inverse-engineering techniques to improve the performance of quantum simulation protocols.

PACS numbers: 37.10.Ty, 03.65.Pm, 03.67.Ac

I. INTRODUCTION

A recent highlight in the remarkable history of the Dirac equation is the realization that non-relativistic systems such as an ultracold trapped ion can obey this equation, with a proper reinterpretation of symbols, under specific trapping conditions and laser interactions. In a one dimensional setting (linear trap), two levels of the ion interacting with laser fields set the basis that spans the relevant internal state subspace, whereas orthogonal eigenvectors of the Dirac Hamiltonian with positive and negative energies correspond to matter and antimatter solutions. Similarly, different elements of the original Dirac equation, such as the mass, or the constant playing the role of speed of light, are mapped to atomic or linear electric fields. These mappings and the controllability of trapped ions have been used to observe experimentally simulations of relativistic effects, like Zitterbewegung, or Klein tunneling. Trapped ions are in fact an example of a wider set of non-relativistic “Dirac systems” that obey a Dirac dynamics, for example in condensed matter, optics, cold atoms, or superconducting circuits.

The new physical platforms for Dirac dynamics are often easier to manipulate than relativistic particles. In trapped ions, for example, the effective (simulated) mass, speed of light, or electric field may be changed in time. This opens prospects for finding and implementing new or exotic effects and carrying out further fundamental studies. It also motivates a search for manipulation protocols to achieve specific goals. Shortcuts to adiabaticity (STA) are a group of techniques to speed up adiabatic methods, possibly following non-adiabatic routes, offer a suitable framework for the task, and example cases have been worked out recently in the domain of the Dirac equation. STA are typically highly flexible so that, apart from speeding up the processes, which may be needed to avoid decoherence, the protocol may satisfy further conditions, such as robustness with respect to noise and/or systematic perturbations. Robust protocols have been demonstrated for the Schrödinger equation and, as we shall see in this paper, can be extended as well to the Dirac equation.

II. DRIVEN DIRAC DYNAMICS WITH TIME-DEPENDENT VECTOR FIELD

We focus now on a 1 + 1-dimensional Dirac equation for a charged particle moving in x-direction, which could be simulated by ultra cold trapped ions and realizes quantum relativistic effects. It may be written as

\[ i\hbar \dot{\Psi}(t) = \left( -i\hbar c \sigma_x + A(x,t) \sigma_z + mc^2 \sigma_z \right) \Psi(t), \]

where \( |\Psi(t)\rangle \) is the two-component time-dependent wave function for the particle with mass \( m \), the dot means time derivative, \( c \) is the speed of light, \( \hbar \) is the Planck constant divided by \( 2\pi \), and \( \sigma_{x,y,z} \) are \( 2 \times 2 \) Pauli matrices in the basis \( |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) and \( |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \). To implement a time-dependent but spatially homogeneous electric field, we set \( A(x,t) \) as a purely time-dependent vector field.
dependent function, \( A(x,t) = \alpha_t \). Then the Hamiltonian reads

\[
H = -i\hbar c \partial_t \sigma_x + \alpha_t \sigma_x + mc^2 \sigma_z. \tag{2}
\]

Beware that \( c, m, \) and the electric field must be reinterpreted in the simulated dynamics, as discussed in \([2, 5]\) and later in Sec. \( \text{VI} \). Note also that, whereas the two components of the state do not represent the spin in the relativistic interpretation \([17]\), the two levels \(|1\rangle\) and \(|2\rangle\) in the simulation simply become two bare internal levels of the ion.

Defner \([12]\) used the fast-forward shortcut technique \([18, 19]\) to suppress “production of pairs” (transitions among positive and negative energy solutions) in fast processes, combining scalar and pseudoscalar potentials. Our goal here is instead to induce a fast and robust population inversion among the bare levels. A different technique will be applied, designing the time dependence of the parameters in the Hamiltonian rather than adding terms to it. This is carried out by making use of invariants of motion twice: first to decompose the solution of the Dirac equation into independent subspaces for each plane wave, and then, to describe and manipulate the solution for the internal state amplitudes within each subspace \([14]\).

### III. SOLUTIONS VIA INVARIANTS

We shall find exact solutions of the Dirac equation in Eq. (1) based on the Lewis and Riesenfeld theory of invariants \([20]\). For the Hamiltonian in Eq. (2), let us assume that a nontrivial invariant exists with the form \([21, 23]\)

\[
I = A(t)p + B(t)x + D(t),
\]

where \( A(t), B(t), \) and \( D(t) \) are \( 2 \times 2 \) matrices. The invariant should satisfy the equation

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

Substituting Eqs. (2) and (3) into Eq. (4) gives

\[
[A, \sigma_x] = 0, \tag{5}
\]

\[
[B, \sigma_x] = 0, \tag{6}
\]

\[
a_1[A, \sigma_x] + mc^2[A, \sigma_x] + \epsilon[D, \sigma_x] + i\hbar A = 0, \tag{7}
\]

\[
a_1[B, \sigma_x] + mc^2[B, \sigma_x] + i\hbar B = 0, \tag{8}
\]

\[
icB\sigma_x + a_1[D, \sigma_x] + mc^2[D, \sigma_x] + i\hbar D = 0. \tag{9}
\]

Expanding the matrices in the \( su(2) \)-basis, \( A = a_1 + a_2 \sigma_x + a_3 \sigma_y + a_4 \sigma_z \), with \( a_i \) an arbitrary real number for \( i = 1, 2, 3, 4 \), and similarly for \( B \) and \( D \), the above equations are easy to solve. From Eqs. (5) and (6), we get

\[
A = a_1 + a_2 \sigma_x, \tag{10}
\]

\[
B = b_1 + b_2 \sigma_x, \tag{11}
\]

where \( a_1, a_2, b_1, b_2 \) are to be determined. Substituting Eq. (10) into Eq. (7), we have

\[
b_1 = b_2 = 0, \tag{12}
\]

\[
b_2 = 0. \tag{13}
\]

Substituting Eq. (11) into Eq. (8), we have

\[
cd_4 = mc^2 a_2, \tag{14}
\]

\[
d_3 = 0, \tag{15}
\]

\[
a_1 = d_3 = 0. \tag{16}
\]

Similarly, from Eq. (9), we find

\[
cb_1 + \hbar d_4 = 0, \tag{17}
\]

\[
a_1 d_4 = mc^2 d_2, \tag{18}
\]

\[
\dot{a}_1 = d_4 = 0. \tag{19}
\]

The invariant can be then written as

\[
I = (a_1 p + b_1 x + d_1) + (a_2 p + d_2) \sigma_x + d_3 \sigma_z, \tag{20}
\]

where \( a_1, b_1, d_1, \) and \( d_2 \) are constant. If \( a_1 \) is time-dependent, then \( d_3 = d_2 = 0, \) and therefore \( b_1 = a_2 = 0 \). The invariant can be simplified as

\[
I = a_1 p + d_1 = a_1(p + \mathbb{C}), \tag{21}
\]

where \( \mathbb{C} \) is a constant. This holds even for a time-dependent mass. Consistently, the Heisenberg equations of motion for the system Eq. (2) are

\[
\frac{dp}{dt} = 0, \quad \frac{dx}{dt} = c \sigma_x. \tag{22}
\]

In other words, the momentum operator is invariant, which may be interpreted as the initial momentum \( p_0 \) \([24]\), as shown below making use of a different frame.

The solutions of the time-dependent Dirac equation may be written as linear superpositions of eigenvectors of the invariant \([20]\). Since the eigenfunctions of the invariant take the plane-wave form \( e^{ip_0 \cdot \mathbf{x}/2} \) with \( p_0 \) a real number, we assume the existence of plane wave solutions of Eq. (2) according to the ansatz

\[
|\psi(t)\rangle = e^{ip_0 \cdot \mathbf{x}/2} |\phi_{p_0}(t)\rangle, \tag{23}
\]

where \( |\phi_{p_0}(t)\rangle \) is a \( 2 \times 1 \) vector that depends on the parameters \( p_0 \) and \( t \).

Substituting Eq. (12) into the time-dependent Dirac equation in Eq. (1) gives the following reduced \( (2 \times 2) \) Dirac equation for the vector \( |\phi_{p_0}(t)\rangle \),

\[
i\hbar |\phi_{p_0}(t)\rangle = H_{p_0} |\phi_{p_0}(t)\rangle, \tag{24}
\]

where

\[
H_{p_0} = cp_0 \sigma_x + a_1 \sigma_x + mc^2 \sigma_z. \tag{25}
\]

By superposing plane wave solutions, general (wave packet) solutions are found, of the form

\[
|\Psi(t)\rangle = \int_{-\infty}^{\infty} a(p_0)|\phi_{p_0}(t)\rangle dp_0, \tag{26}
\]

where each (momentum) component evolves with its own \( 2 \times 2 \) Hamiltonian \( H_{p_0} \), so that the corresponding global (wave packet) populations for \( |1\rangle \) and \( |2\rangle \) are given by

\[
P_k = \int_{-\infty}^{\infty} |a(p_0)|^2 P_k(p_0) dp_0, \tag{27}
\]
where \( k = 1, 2 \) and \( P_k(p_0) = |(k|\phi_{p_0}(t))|^2 \) \((k = 1, 2)\) are the populations for each momentum in the basis \([1], [2]\). In the numerical examples we take a Gaussian function \(|a(p_0)|^2 = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-p_0^2/\sigma^2)\).

The homogeneous electric field is more often represented by a linear scalar potential. To find this representation and see the equivalence with our treatment, we change the frame by means of the unitary transformation \( U = e^{-i\alpha(t)/\hbar c} \). The effective Hamiltonian becomes

\[
H_u = U^\dagger H U - i\hbar U^\dagger U = c p e x + m e^2 \frac{x}{2} - \alpha t x / c, \tag{24}
\]

where we have used the Hausdorff expansion, which can be truncated here exactly, as \( e^{i e x} e^{-i e x} = H + \xi [x, H], \) with \( \xi = -i\alpha t / (\hbar c) \). The homogeneous field is now represented by a linear scalar potential of time-varying slope. The plane wave solutions transform as \( |\phi_x(t)\rangle = U^\dagger |\phi(t)\rangle = e^{i(\rho_0 + \rho_i x / \hbar c)} |\phi_{p_0}(t)\rangle \) so they get a time-dependent momentum and the invariant of \( H_0 \) becomes (as it may be seen by repeating the steps after Eq. (4) for \( H_u \)). Since the two frames are unitarily connected, in what follows we shall use for simplicity the one based on \( H \).

IV. ROBUST QUANTUM STATE ENGINEERING

A. Invariant-based shortcuts to adiabaticity for driven Dirac dynamics

The Hamiltonian \( H_{p_0} \) in (21) for the Dirac system with spatially homogeneous electric field reads in matrix form

\[
H_{p_0} = \begin{pmatrix}
mc^2 & cp_0 + \alpha t \\
 cp_0 + \alpha t & -mc^2
\end{pmatrix}. \tag{25}
\]

If the functions of time \( m(t) \) and \( \alpha \) are given, different values of \( p_0 \) imply different \( 2 \times 2 \) Hamiltonians, with different solutions of the Dirac equation (23). If we design \( m(t) \) and \( \alpha \) by inverse engineering so as to induce a population inversion (or some other operation), say at \( p_0 = 0 \), which we assume to be the average momentum of a wave packet, the solution for any other momentum will generally fail to satisfy the intended task. In other words, the spread of \( p_0 \) in a wave packet can affect the dynamics and induce errors. Therefore, it is necessary to design protocols robust with respect to the momentum spread. The perturbed Hamiltonian \( H_{p_0} \) can be decomposed as \( H_{p_0} = H_0(t) + H_1(t) \), where \( H_0(t) = \begin{pmatrix}
mc^2 & \alpha t \\
 \alpha t & -mc^2
\end{pmatrix} \) is the unperturbed Hamiltonian and \( H_1(t) = \begin{pmatrix}
0 & p_0 \\
 p_0 & 0
\end{pmatrix} \) is the “systematic error” Hamiltonian. In the following, adopting the standard notation for two-level Hamiltonians in quantum optics, \( \frac{\Delta}{2} \alpha \) for \( A(t) = mc^2 \) and \( \frac{\Delta}{2} \Omega(t) = \alpha, \) in terms of a detuning \( \Delta \), and a Rabi frequency \( \Omega \), we write

\[
H_0(t) = \frac{\hbar}{2} \begin{pmatrix}
\Delta & \Omega \\
\Omega & -\Delta
\end{pmatrix}. \tag{26}
\]

The instantaneous adiabatic eigenstates of \( H_0(t) \) are

\[
|E_+(t)\rangle = \cos \left( \frac{\varphi}{2} \right) |1\rangle + \sin \left( \frac{\varphi}{2} \right) |2\rangle, \tag{27}
\]

\[
|E_-(t)\rangle = \sin \left( \frac{\varphi}{2} \right) |1\rangle - \cos \left( \frac{\varphi}{2} \right) |2\rangle, \tag{28}
\]

with the mixing angle \( \varphi = \arctan(\Delta / \Omega) \) and the corresponding adiabatic energies \( E_\pm(t) = \pm \frac{\hbar}{2} \sqrt{\Delta^2 + \Omega^2} \).

For this time-dependent \( 2 \times 2 \) Hamiltonian \( H_0 \), there exists a dynamical invariant \( I_0 \), not to be confused with the momentum invariant of Eq. (2). This invariant in the internal-state subspace can be written as \( I_0 = \text{Tr} (|1\rangle \langle 1| H \Omega) \).

\[
I_0(t) = \frac{\hbar}{2} \Omega_0 \left( \cos \theta \sin \theta e^{i\beta} - \cos \theta \right), \tag{29}
\]

where \( \Omega_0 \) is an arbitrary constant (angular) frequency to keep \( I_0(t) \) with dimensions of energy, and \( \theta \) and \( \beta \) are auxiliary time-dependent angles. Using Eqs. (26) and (29) in Eq. (4) we find the differential equations

\[
\dot{\theta} = \Omega \sin \beta, \tag{30}
\]

\[
\dot{\beta} = \Omega \cot \theta \cos \beta - \Delta. \tag{31}
\]

The eigenstates of the invariant are

\[
|\phi_+(t)\rangle = \left( \begin{array}{c}
\cos (\theta/2) e^{i\beta/2} \\
\sin (\theta/2) e^{-i\beta/2}
\end{array} \right), \tag{32}
\]

\[
|\phi_-(t)\rangle = \left( \begin{array}{c}
\sin (\theta/2) e^{i\beta/2} \\
-\cos (\theta/2) e^{-i\beta/2}
\end{array} \right) \tag{33}
\]

which satisfy \( I_0|\phi_{p_0}(t)\rangle = \lambda_n|\phi_{p_0}(t)\rangle \) \((n = \pm)\) with the eigenvalues \( \lambda_\pm = \pm \hbar \Omega_0/2 \). The general solution of the time-dependent Schrödinger equation, according to the theory of Lewis and Riesenfeld [20], can be written as a linear combination \( |\Phi_\alpha\rangle = \sum_n c_n e^{i\phi_n}|\phi_n\rangle \), where \( c_n \) are time-independent amplitudes, and the \( \epsilon_n \) are the Lewis-Riesenfeld phases

\[
\epsilon_n = \frac{1}{\hbar} \int_0^t \left( \dot{\phi}_n(t') - \frac{\partial}{\partial t'} \right) dt'. \tag{34}
\]

Then, two orthogonal solutions can be constructed as

\[
|\psi_0(t)\rangle = e^{-i\gamma/2} |\phi_+(t)\rangle = e^{-i\gamma/2} \left( \begin{array}{c}
\cos (\theta/2) e^{i\beta/2} \\
\sin (\theta/2) e^{-i\beta/2}
\end{array} \right) \tag{35}
\]

and

\[
|\psi_-(t)\rangle = e^{i\gamma/2} |\phi_-(t)\rangle = e^{i\gamma/2} \left( \begin{array}{c}
\sin (\theta/2) e^{i\beta/2} \\
-\cos (\theta/2) e^{-i\beta/2}
\end{array} \right) \tag{36}
\]

where \( \gamma = 2 \epsilon_\alpha = -2 \epsilon_\alpha \) and \( \langle \psi_{p_0}(t)|\psi_{p_0}(t)\rangle = 0 \) for all times. Thus, by using Eqs. (20) and (24), we find

\[
\gamma = \frac{\Omega \cos \beta}{\sin \theta} = \frac{-\dot{\theta} \cos \beta}{\sin \theta \sin \beta}. \tag{37}
\]

Our aim is to design invariant-based shortcuts to achieve a population inversion from state \( |1\rangle \) to state \( |2\rangle \), up to a global phase factor, along the invariant eigenstate \( |\phi_+(t)\rangle \) in a given
time \( t_f \). We therefore write down the boundary conditions for \( \theta \) to guarantee the desired initial and final states,

\[
\theta(0) = 0, \quad \theta(t_f) = \pi. \quad (38)
\]

In addition, if we impose \([H_0(0), I_0(0)] = 0\) and \([H_0(t_f), I_0(t_f)] = 0\) so that the Hamiltonian \( H_0(t) \) and the invariant \( I_0(t) \) share common eigenstates at initial and final times, we have the following additional boundary conditions,

\[
\Omega(0) = 0, \quad \dot{\Omega}(0) = 0, \\
\Omega(t_f) = 0, \quad \dot{\Omega}(t_f) = 0. \quad (39)
\]

The Rabi frequency and detuning leading to a fast population inversion are determined from Eqs. (30) and (31), choosing a convenient function of \( \beta \), and interpolating \( \theta \) to satisfy the boundary conditions (38) and (39).

**B. Robust shortcuts against systematic momentum errors**

![Graph showing q_s vs. \( \nu \)](image)

**Fig. 1:** (Color online) Systematic error sensitivity \( q_s \) in Eq. (43). As in all figures we use dimensionless units with \( c = \hbar = t_f = 1 \). For specific values of \( |\nu| \), \( q_s \) is 0 is satisfied, in particular at the minimal value \( |\nu| = 0.643 \).

To construct invariant-based shortcuts robust against the systematic momentum errors, we use perturbation theory up to \( O(p_0^0) \) to find the time evolution of the quantum state governed by \( H_{p_0} \) that starts as \( |\psi(0)\rangle \),

\[
|\psi(t_f)\rangle = |\psi(0)\rangle + \frac{i}{\hbar} \int_0^{t_f} dt \hat{U}_0(t_f, t) H_1(t) |\psi(0)\rangle \\
- \frac{1}{\hbar^2} \int_0^{t_f} dt \int_0^{t_f} dt' \hat{U}_0(t, t') H_1(t') |\psi(0)\rangle + \cdots, \quad (40)
\]

where \( |\psi(t)\rangle \) is the unperturbed solution and \( \hat{U}_0(s, t) = |\psi_0(s)\rangle \langle \psi_0(t)| + |\psi_\perp(s)\rangle \langle \psi_\perp(t)| \) is the unperturbed time evolution operator. We assume that the error-free \( (p_0 = 0) \) scheme works perfectly, i.e., \( |\psi(0)\rangle = |1\rangle, |\psi(t_f)\rangle = |2\rangle \). Then, the probability of the excited state at the final time for \( t_f \) and momentum \( p_0 \) is

\[
P_2(p_0) = |\langle \psi(0)|\psi(t_f)\rangle|^2 = 1 \left( - \frac{1}{\hbar^2} \int_0^{t_f} dt \langle \psi_\perp(t)|H_1(t)|\psi_\perp(t)\rangle \right)^2. \quad (41)
\]

Defining the systematic error sensitivity as \([15, 16]\)

\[
q_s := \frac{-1}{\hbar^2} \frac{\partial^2 P_2(p_0)}{\partial p_0^2} \bigg|_{p_0=0} = - \frac{\partial P_2(p_0)}{\partial p_0^2} \bigg|_{p_0=0}, \quad (42)
\]

we have

\[
q_s = \frac{c^2}{\hbar^2} \left| \int_0^{t_f} dt e^{-i\gamma} (-i \sin \beta - \cos \theta \cos \beta) \right|^2. \quad (43)
\]

For a flat \( \pi \) pulse, \( \beta = \pi/2 \), and \( \theta = \pi t_f/\Omega \), so \( \dot{\theta} = \pi/t_f, \Omega = \pi t_f, \Delta = 0 \), and \( \gamma = 0 \). This gives

\[
q_s(\pi \text{ pulse}) = \frac{c^2 t_f^2}{\hbar^2}. \quad (44)
\]

Optimally robust invariant-based shortcuts are now defined as those that make the systematic error sensitivity zero. Following [27], we could try the simple Fourier series type of ansatz

\[
y = 2\theta + \nu \sin(2\theta), \quad (45)
\]

where \( \nu \) is a real number that may be varied to nullify \( q_s \). (It is possible to extended this ansatz to make further derivatives zero as in [27].) Alternatively we use [15]

\[
y = \nu[2\theta - \sin(2\theta)]. \quad (46)
\]

Both ansatzes are valid and nullify \( q_s \) for different values of \( \nu \). They lead approximately to the same pulse area \( A = \int_0^{t_f} \Omega(t) dt \), but the second one provides simpler expressions of \( \beta, \Omega \) and \( \Delta \), using Eqs. (30), (31), and (37), so it is preferred here. Specifically, using Eqs. (37) and (46), the parameter \( \beta \) takes the form

\[
\beta = \arccot(4\nu \sin^3 \theta). \quad (47)
\]

This gives \( \beta(0) = \beta(t_f) = \pi/2 \) so that the invariant eigenstate \( |\phi_\nu(t)\rangle \), see Eq. (42), evolves from \( |1\rangle \) to \( |2\rangle \) up to phase factors, \( |\phi_\nu(0)\rangle = e^{i\nu \theta/4}|1\rangle \) and \( |\phi_\nu(t_f)\rangle = e^{-i\nu \theta/4}|2\rangle \). Finally, the systematic errors sensitivity is given by

\[
q_s = \frac{c^2}{\hbar^2} \left| \int_0^{t_f} dt e^{-i(\nu[2\theta - \sin(2\theta)] - 4\nu \sin^3 \theta \cos \theta)} \right|^2 \frac{1}{1 + 16\nu^2 \sin^2 \theta}. \quad (48)
\]

Fig. 1 shows the systematic error sensitivity versus \( \nu \), passing through zeroes of \( q_s \). (In all numerical calculations we use dimensionless units with \( c = \hbar = t_f = 1 \). The dimensionless effective mass generally depends on time so it is not made one as usual.) The corresponding Rabi frequency and detuning are

\[
\Omega = \dot{\theta} \sqrt{1 + 16\nu^2 \sin^2 \theta}, \quad (49)
\]

\[
\Delta = 16\nu \sin^2 \theta \cos \theta \theta \frac{1 + 4\nu^2 \sin^6 \theta}{1 + 16\nu^2 \sin^2 \theta}. \quad (50)
\]

\( \Omega \) increases monotonously with \( \nu \) so we choose the smaller value consistent with \( q_s = 0 \), \( \nu_m = 0.643 \), to minimize \( \Omega \) along the evolution path. In addition, to interpolate at intermediate times, we assume a polynomial ansatz \( \theta = \sum_{j=0}^3 a_j \nu^j \), where
the coefficients \(a_i\) are found by solving the equations set by the boundary conditions on \(\theta\) and its derivative, see Eqs. (38) and (39). The time-dependent \(\Omega\) and \(\Delta\) are shown in Fig. 2 (a), with absolute value maxima \(|\Omega_m| \approx 13\) and \(|\Delta_m| \approx 10\). For the specified \(H_0(t)\) in Eq. 26, corresponding to \(p_0 = 0\), we solve \(H_0 |\phi_0(t)\rangle = i\hbar |\phi_0(t)\rangle\) numerically by a Runge-Kutta method with an adaptive step, and get the time evolution of the populations \(P_\pm(p_0 = 0)\) for the optimal protocol represented in Fig. 2(a). Fig. 2(b) shows the population inversion between \(|1\rangle\) and \(|2\rangle\). By contrast, solving the dynamics separately for each \(p_0\) with \(H_{\text{opt}}\), and averaging the populations \(P_\pm(p_0)\) according to Eq. 23, Fig. 3 shows the change of the global population \(P(t)\) for Gaussian wave packets with \(\sigma = 0.3\) and \(\sigma = 0.9\), respectively. The population inversion is still accurate for \(\sigma = 0.3\), but by further increasing the momentum width, it eventually must fail. \(P_\pm(p_0)\) is shown in the next section, making explicit the momentum-width window where a perfect inversion can be achieved.

![Fig. 2](image2.png)  
**FIG. 2:** (Color online) (a) The Rabi frequency \(\Omega\) (red, solid line) and detuning \(\Delta\) (blue, dotted-dashed line) in our optimal protocol. (b) Time evolution of the populations \(P_\pm(0)\) (blue, solid line) and \(P_\mp(0)\) (red, dotted-dashed line) during the population inversion. We have used \(\nu = 0.643\) and \(p_0 = 0\).

![Fig. 3](image3.png)  
**FIG. 3:** (Color online) Time evolution of the populations \(P_\pm\) of a Gaussian wave packet centered at zero momentum (green, solid line and blue, dot-dashed line for \(\sigma = 0.3\) and \(\sigma = 0.9\), respectively) and \(P_\mp\) (red, dotted-dashed line and black circles for \(\sigma = 0.3\) and \(\sigma = 0.9\), respectively) by averaging over all momenta \(p_0\), see Eq. 23, during the population inversion. \(H_0\) as in Fig. 2(a). Compare to the result for a plane wave, \(p_0 = 0\), in Fig. 2(b).

We plot the adiabatic (instantaneous) eigenenergies of \(H_0(t)\) in Fig. 4(a) for the optimal protocol. Note the degeneracy at the edge times due to the vanishing of \(\Delta\) and \(\Omega\). Fig. 4(b) depicts the adiabatic time evolution of the populations of level \(|1\rangle\) in both eigenstates, \(|\langle 1|E_\alpha(t)\rangle|^2\) and \(|\langle 1|E_\beta(t)\rangle|^2\). In addition, Fig. 5 depicts the instantaneous populations of positive and negative energy eigenstates for the invariant eigenstates, \(|\langle E_\alpha(t)|\phi_\alpha(t)\rangle|^2\) and \(|\langle E_\beta(t)|\phi_\beta(t)\rangle|^2\). While the positive energy solution dominates most of the time, both are equally important at boundary times.

![Fig. 4](image4.png)  
**FIG. 4:** (Color online) (a) The adiabatic energies of Hamiltonian \(H_0(t)\): \(E_\alpha(t)\) (red, solid line) and \(E_\beta(t)\) (blue, dotted-dashed line). (b) The adiabatic time evolution of the populations of level \(|1\rangle\) for the positive (red, solid line) and negative (blue, dotted-dashed line) energy eigenstates of Hamiltonian \(H_0(t)\). \(\Omega\) and \(\Delta\) are as in Fig. 2(a).

![Fig. 5](image5.png)  
**FIG. 5:** (Color online) Populations of energy eigenstates along the invariant eigenstate \(|\phi_\alpha(t)\rangle\), \(|\langle E_\alpha(t)|\phi_\alpha(t)\rangle|^2\) (red, solid line) and \(|\langle E_\beta(t)|\phi_\beta(t)\rangle|^2\) (blue, dotted-dashed line), for the optimal \(\Omega(t)\) and \(\Delta(t)\) in Fig. 2(a).

V. ROBUSTNESS AGAINST WAVE PACKET MOMENTUM SPREAD

We now test the stability of the optimal invariant-based protocol of the previous section with respect to the momentum spread in wave packets, compared to a simple invariant-based shortcut for which the sensitivity is not zero. Both protocols should invert the population along the invariant eigenstate \(|\phi_\alpha(t)\rangle\) in a given time \(T_f\) for \(p_0 = 0\). Let us denote by a subscript “s” the auxiliary angles \(\theta_s(t)\) and \(\beta_s(t)\) and the Hamiltonian functions \(\Omega_s\), \(\Delta_s\) for the simple protocol with nonzero sensitivity. To perform a fair comparison, we impose the same maxima of Rabi frequency and detuning for the two protocols. We also take \(\theta_s(t) = \theta(t)\) and \(\beta_s(0) = \beta_s(T_f) = \pi/2\) for simplic-
Fig. 6: The Rabi frequency $\Omega_r$ (green, dotted-star line), and detuning and $\Delta_r$ (black, dashed line) are determined by Eqs. (20) and (31) with angles $\theta_s(t) = \sum_{s=0}^{+} a_s t^i$ and $\beta_s(t) = \sum_{s=0}^{+} b_s t^i$ in simple invariant-based shortcuts, together with “optimal” $\Omega(t)$ (red, solid line) and $\Delta(t)$ (blue, dotted-dashed line) in Fig. 2(a).

Fig. 7: Probability $P_{\Omega}(p_0)$ at the final time $t_f = 1$ versus systematic momentum noise $p_0$ by solving numerically Eq. (20) with the Hamiltonian [25] based on the optimal invariant-based shortcut of Fig. 2(a) (zero sensitivity, red, solid line), and simple ones (nonzero sensitivity, blue, dotted-dashed line).

VI. TRAPPED-ION IMPLEMENTATION

Even though the basic structure of a trapped-ion implementation of a 1+1 Dirac equation was already proposed in Refs. [3–5], in our current formalism the simulated mass and electric field should be time-dependent and highly controllable, which is a novelty with respect to previous Dirac equation proposals and experiments in trapped ions. The high degree of laser control in trapped ions enables this kind of approach, given that laser amplitudes can be turned on and off in situ and their profiles designed according to the requirements of the proposed protocol.

In the Lamb-Dicke regime, the Hamiltonian describing the carrier interaction of a pair of internal levels of a single ion with mass $M$ driven by a laser field takes the form of $H_c = \hbar \Omega (\sigma^x e^{i \phi} + \sigma^- e^{-i \phi})$, where $\eta = k \sqrt{\hbar/2 M v_0}$ is the Lamb-Dicke parameter [28, 29] with $k$ the wave number of the driving field and $v_0$ the frequency of a center-of-mass mode, $\Omega$ is the Rabi frequency, $\phi$ is the field phase, and $\sigma^+ (\sigma^-)$ is the raising (lowering) ionion spin-1/2 operator. A Jaynes-Cummings (JC) Hamiltonian, also known as red-sideband interaction, $H_r = \hbar \Omega \eta (\sigma^x e^{i \phi} + \sigma^- a e^{-i \phi})$, couples the two internal levels of the ion and one of the vibrational center-of-mass modes, where $a (a^\dagger)$ is the annihilation (creation) operators of the vibrational mode. In the blue motional sideband, also known as anti-JC (AJC) interaction, the Hamiltonian can be written as $H_b = \hbar \Omega \eta (\sigma^+ a e^{i \phi} + \sigma^- a^\dagger e^{-i \phi})$, where $\Omega_r(b)$ are the Rabi frequency and phase of the light field. By applying all of these interactions simultaneously with appropriate Rabi frequencies and relative phases, the Dirac Hamiltonian for a free particle, $H_{\text{free}} = c r \cdot p + m c^2 \gamma_z$, can be completely mapped by making the identifications $m c^2 := \hbar \omega_c$, and $c := \sqrt{2 \eta / \Omega_1 + \Omega_r}$ [3, 4]. Here, $p = i \hbar (a^\dagger - a)/2 \Lambda$ with $\Lambda = \sqrt{\hbar/4 M v_0}$ the size of zero-point wave packet, and $\Omega_1 = \Omega_r$. We point out that the carrier can generate a mass term with $\sigma_z$. Pauli matrix at lowest order, which contains the same physics as the $\sigma_z$. Given that the same Clifford algebra is satisfied. Another possibility that does not employ the carrier is via a detuning in the red and blue sideband pulses, which will directly generate the $\sigma_z$ term in an appropriate interaction picture. In general, a time-dependent Rabi frequency $\Omega_c$ or detuning will induce a simulated time-dependent mass in the Dirac system, as our protocol does. In addition, as shown in [4], a free Dirac equation can be encoded by a single ion (ion 1), and external potentials can be implemented by a second ion (ion 2) driven by another bichromatic light field with same vibrational mode but a different electronic transition. For example, by imposing a laser field with appropriate phases and a time-dependent Rabi frequency $\Omega_2$ on the ion 2, the Hamiltonian for the two-ion system will take the form of $H_2 = c r \cdot p + m c^2 \gamma_z e^{i \phi_2}$, where $-e$ is the electron charge, $\phi_2$ is a nonzero electric potential, $e \phi_2 := g(t) \sigma_z x$.
with \( g(t) = \hbar \langle \tilde{\psi}_2(t) \rangle / \Lambda \), and \( x = (a + a^\dagger) \Lambda \) is the position operator [5]. If ion 2 is prepared in the positive eigenstate of Pauli operator \( \sigma_x^{(2)} \), this operator could be replaced by its +1 eigenvalue, and this reduces to a linear potential in the Hamiltonian \( H_n \), which is in consistent with the Hamiltonian \( H_n \) in Eq. (24), with \( \alpha_t / c := g(t) \). Up to a unitary transformation \( \mathcal{U}^\dagger = e^{-i x / \hbar} \), the Hamiltonian \( H \) of Eq. (2) is found. Thus, the optimal robust quantum state engineering protocol in Dirac dynamics can be effectively mapped by a string of two trapped ions. Alternatively, the synthetic electric field may be implemented directly in \( H \) without a second ion with a proper pulse. Unlike the Schrödinger equation, a \( \pi \)-carrier pulse for Dirac dynamics does not invert the population perfectly for a wave packet, see Eq. (44), due to the first term in \( H \), a problem that may be solved by inverse-engineered optimized pulses as the ones proposed in Sec. IV.

VII. DISCUSSION AND SUMMARY

Different systems that behave according to the same model equations—with disparate interpretation of the symbols—simulate each other. Often one of these systems is easier to control and manipulate. It may also obey the model for a domain of parameters hard or impossible to implement in the other one leading to exotic phenomena. Dirac systems obeying the Dirac equation represent well this scenario and offer manipulation possibilities much beyond the ones for the domain of spin-1/2 relativistic particles. In line with the current interest to develop quantum technologies, quantum effects beyond the Schrödinger equation, as those described by a Dirac equation, are being investigated due to peculiarities of the spectrum, band structure, rich phase diagrams, remarkable transport properties \([2, 3, 5]\), and control possibilities implied by the coupling between internal states and momentum \([32]\). This motivates the development of efficient control approaches for Dirac dynamics. The mentioned coupling may be useful for well defined momenta, but also limits the controllability of internal states introducing systematic errors for a wave packet with a nonnegligible momentum width. We have demonstrated that inverse engineering based on invariants of motion provides robust protocols for manipulating the qubit in a 1+1 Dirac system implemented by trapped ions. This example suggests that “shortcuts to adiabaticity” are a useful tool in the broad context of quantum simulations and more generally to develop quantum technologies.

ACKNOWLEDGMENTS

The authors acknowledge support from Spanish MINECO/FEDER Grants FIS2015-69983-P, FIS2015-67161-P, Basque Government Grant IT986-16, Ramón y Cajal Grant RYC-2012-11391, UPV/EHU UFI 11/55, National Natural Science Foundation of China under Grant No. 11674033 and No. 11474026, and the Fundamental Research Funds for the Central Universities under Grant No. 2015KJJCA01.
[32] J. Schliemann, D. Loss, and R. M. Westervelt, Phys. Rev. Lett. 94, 206801 (2005).