Multiple Schrödinger pictures and dynamics in shortcuts to adiabaticity

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A Schrödinger equation may be transformed by unitary operators into dynamical equations in different interaction pictures which share with it a common physical frame, i.e., the same underlying interactions, processes and dynamics. In contrast to this standard scenario, other relations are also possible, such as a common interaction-picture dynamical equation corresponding to several Schrödinger equations that represent different physics. This may enable us to design alternative and feasible experimental routes for operations that are a priori difficult or impossible to perform. The power of this concept is exemplified by engineering Hamiltonians that improve the performance or make realizable several shortcuts to adiabaticity.

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Introduction.—Schrödinger, Interaction, or Heisenberg “representations” or “pictures” of a quantum system are linked to each other by unitary transformations that guarantee their formal equivalence. Changing the picture may be viewed as a change of basis, so in principle the same information can be extracted from any of them. This fundamental equivalence is compatible with distinguishing features, for example with respect to their usefulness (\(i\)) to calculate, approximate, or modify the dynamics, and (\(ii\)) to describe the system, its properties, and their closeness or otherwise to common language or classical notions. The Schrödinger picture (SP) is often privileged as the primary description, representative of the physical or experimental setting, whereas the multiple interaction pictures (IP) have the connotation of auxiliary mathematical constructs to facilitate the calculations. The standard relation among them is schematically depicted in Fig. 1(a), where each node may represent the dynamical equations (DE) for state vectors, the Hamiltonians, or the state vectors themselves. The external box means that they all represent the same common underlying physics: the same interactions and external forces, and the same system dynamics ("physical frame" for short).

In sharp contrast to the common wisdom scenario we have just described, we propose in this letter alternative relations such as the ones in Figs. 1(b), 1(c) or more complex combinations, where the nodes may belong to different physical frames, as a way to design alternative and feasible experimental routes for operations that are a priori difficult or impossible to perform. This will be applied in particular to engineer Hamiltonians which improve or make feasible “shortcuts to adiabaticity” \([1]\). Adiabatic processes are very common and useful in laboratories, but their intrinsic slowness imposes limitations. The design of alternative fast routes is an active research field of interest in cold atom physics, nuclear magnetic resonance, quantum information processing, and beyond the quantum domain, e.g. to couple different devices in optical communications \([2]\). Shortcuts designed on paper, may or may not be feasible in practice, so the possibility to generate multiple physical frames proves useful. Our first benchmark problem is the acceleration of adiabatic population inversion in a two-level system, in itself a phenomenon of broad interest from NMR applications \([3]\) to quantum information \([4]\). We shall point out several techniques to eliminate undesired Hamiltonian terms, possi-
ouble improvements to reinterpreted experiments, and also feasible alternatives to inversion schemes that required cumbersome level-shift engineering or multiple fields [5]. We shall finally show how to overcome the difficulties to implement “counterdiabatic” terms and perform fast compressions or expansions of cold atoms without final excitation [6].

Multiple Schrödinger pictures. — To explain the multi-frame schemes of Figs. 1(b) and 1(c) we need first to review some basic equations and notation. SP and IP states are related by a unitary transformation, $|ψ_I⟩ = U^t|ψ_S⟩$, $|ψ_S⟩ = U|ψ_I⟩$, and evolve according to

$$iℏ\partial_t|ψ_S⟩ = H|ψ_S⟩, \quad iℏ\partial_t|ψ_I⟩ = H_I|ψ_I⟩,$$  \hspace{1cm} (1)

where $H$ is the Hamiltonian in the SP and $H_I = U^t(H - K)U$, with $K = ℏU\dot{U}^t$, the corresponding IP Hamiltonian. Note that $H$, $H_I$ and $K$ may be generally time-dependent. Similar relations hold for a unitary operator $U'$ which defines an interaction picture $^I$. As in Fig. 1(b), an interaction picture DE may be related unitarily to two or more Schrödinger equations with Hamiltonians that represent different experimental settings and external interactions. There is no contradiction with the equivalence discussed above when we pay attention, not only to the DEs but to the observables as well. A given picture is fully characterized by both the DE and the operators for the observables. Thus Fig. 1(b) admits several interpretations depending on the treatment given to the observables: If the observables are transformed, from $B_S$ in $S$ to $B_{S'} = U'^tU^tB_SU^t$ in $S'$, we will get the same expectation values from two different systems and dynamics performing in general rather different measurement operations. If instead one runs the same measurements in $S$ and $S'$ on the same, untransformed observables $B_S$, the expectation values will differ in general, and their IP representatives would be either $U^tB_SU$ or $U'^tB_{S'}U'$, sharing in any case a common IP-state dynamics. It may also occur that, having applied the transformations, the equality $B_{S'} = B_S$ holds for specific (but not for all) observables, as in several examples below.

Another multi-frame scheme is depicted in Fig. 1(c). In the upper box a Schrödinger node is related unitarily to a first IP-node, $I_1$, linked also unitarily to a second one, $I_2$. The two consecutive IP Hamiltonians may be modified or perturbed, e.g. by the addition of some terms (dashed lines). This changes the physics into $^I$ and $^I''$, each in a different physical frame (middle and lower horizontal boxes) with corresponding Schrödinger dynamics. In the example below the consecutive IPs are generated by means of adiabatic and superadiabatic iterations [4, 8], and the addition of a “counterdiabatic” term in the Hamiltonian is performed so as to avoid transitions, canceling out the $K$ in Eq. (2) [4]. This enables us to accelerate slow processes without inducing any final excitation.

Superadiabatic iterations and counterdiabatic corrections. — Our starting model Hamiltonian is

$$H_I(t) = \left( \begin{array}{cc} X_I(t) & \frac{X_I(t) - iY_I(t)}{Z_I(t)} \\ \frac{X_I(t) + iY_I(t)}{Z_I(t)} & -Z_I(t) \end{array} \right) \hspace{1cm} (3)$$

for $j = 0$ and $Y_0 = 0$, i.e., $H_0 = X_0σ_x + Z_0σ_z$ in terms of Pauli matrices. It could represent several physical systems such as a spin in a magnetic field, a two-level atom, or a condensate in the bands of an accelerated optical lattice [10, 11]. In the later case, $X_0$ may be controlled by the trap depth, $Z_0$ by the lattice acceleration [10], and a $Y_0$ component could in principle be implemented by a second shifted lattice [11]. The index $j$ will be used later to define a series of IP Hamiltonians in successive iterations. The Hamiltonian evolution or “trajectory” is here specified by the Cartesian coordinates $X_j, Y_j, Z_j$. Later we shall also use the corresponding polar, azimuthal, and radial spherical coordinates, $Θ_j, Φ_j$, and $R_j$. The radius $x$ may or may not be constant with respect to time, so the trajectory is not generally on a sphere. The Hamiltonian matrices are expressed in the “bare basis” of the two-level system, $|1⟩ = (1, 0), |2⟩ = (0, 1)$. We assume that this is also the eigenbasis of $H_I(t)$, or very close to it for computational purposes, at initial and final times $t = 0$ and $t = t_f$.

Focusing by now on $j = 0$, an adiabatic population inversion is achieved with $H_0$ by varying slowly $X_0$ and $Z_0$ so that the resonance is crossed at $Z_0 = 0$, and the eigenvectors of $H_0$ interchange their character. Different schemes, such as Landau-Zener (LZ), Allen-Eberly [12], and others, may be followed to specify the time-dependences.

The first IP that we shall consider depends on the adiabatic basis $\{|n_0(t)⟩\}$ that diagonalizes $H_0(t)$ and keeps $K(t)$ non-diagonal. Specifically we use $U = A_0$,

$$A_0(t) = \sum_{n=1.2} |n_0(t)⟩⟨n_0(0)|, \hspace{1cm} (4)$$

where we assume that the $|n_0(0)⟩$ coincide with the bare basis. The corresponding $K$ operator in Eq. (2) is denoted as $K_0$. Also, $|ψ_{t_1}⟩ = A_0^†|ψ_S⟩$ and $H_1 = A_0^†(H_0 - K_0)A_0$. Constructing $\{|n_0(t)⟩\}$ requires a proper choice of phases. From an arbitrary adiabatic basis $\{|n_a(t)⟩\}$ that diagonalizes $H_0$ with eigenvalues $E_n(t)$,

$$|n_0(t)⟩ = e^{Γ_n} |n_a(t)⟩,$$  \hspace{1cm} (5)

where $γ_n = i\int_0^t dt'⟨n_a(t')|n_a(t')⟩$ is the geometric phase and the dot denotes time derivative. This phase choice is privileged since $⟨n_0(t)|n_0(t)⟩ = 0$. It also makes $K_0$ non-diagonal and minimizes its norm [5, 13]. In terms of the polar angle $Θ_n$,

$$K_0 = iℏ\dot{A}_0A_0^† = ℏ(\dot{Θ}_0/2)σ_y.$$  \hspace{1cm} (6)
The adiabatic approximation neglects $K_0$ in the IP Hamiltonian $H_1$ to trivially solve
\begin{equation}
\tag{7}
i\hbar \partial_t |\psi_{1t}\rangle = A_{1t}^0 H_0 A_0 |\psi_{1t}\rangle,
\end{equation}
an uncoupled system in the bare basis. Alternatively one may add $A_{1t}^0 K_0 A_0$ to $H_1$ if the effect is to cancel any coupling so that Eq. (7) becomes exact rather than an approximation. In the corresponding SP $S''$, see the middle box in Fig. 1(c), this amounts to adding the counterdiabatic term $H_{cd}^{(0)} := K_0$ to $H_0$. $H_0 + K_0$ preserves the populations of the approximate adiabatic dynamics even for short process times.

In a new iteration, and similarly for higher orders, we write $H_1 = A_{1t}^0 (H_0 - K_0) A_0$ in the form of Eq. (3), $j = 1$, and diagonalize it to produce a “superadiabatic” basis $\{|n_1(t)\}\rangle$, and the transformation
\begin{equation}
\tag{8}
A_1 = \sum_{n=1,2} |n_1(t)\rangle \langle n_1(0)|.
\end{equation}
As before we assume that this basis coincides at the boundary times with the bare basis and that $K_1 = \hbar A_1 A_1^\dagger$ is non diagonal in $\{|n_1(t)\}\rangle$. $A_1$ produces a new IP ($I_2$ in Fig. 1(c)) with $|\psi_{12}\rangle = A_{12}^0 |\psi_{11}\rangle$, and Hamiltonian $H_{cd} = A_{12}^\dagger (H_1 - K_1) A_1$. $K_0$ can be either neglected to produce a superadiabatic approximation, or canceled by adding a counterdiabatic term. In the corresponding SP ($S''$ in Fig. 1(c)) the Hamiltonian becomes $H_0 + H_{cd}^{(1)}$, where $H_{cd}^{(1)} = A_0 K_1 A_0^\dagger$. In that manner a different shortcut Hamiltonian is created. For our reference Hamiltonian $H_0$ with $Y_0 = 0$, and using polar angles for $H_0$ and $H_1$,
\begin{equation}
\tag{9}
H_{cd}^{(1)} = \hbar (\dot{\Theta}_1/2) (\cos \Theta_0 \sigma_x - \sin \Theta_0 \sigma_z),
\end{equation}
if $\Theta_0 < 0$. The absence of a $Y \sigma_y$ component, like in $H_0$ and unlike $H_{cd}^{(0)}$, is in some applications a practical advantage. For example, in an optical lattice implementation of the two-level system only one optical lattice is required: and in a two-level atom realization, discussed below, it avoids the application of a second laser. One more advantage of the superadiabatic shortcut is that $H_{cd}^{(1)}$ is less intense (it has a smaller norm) than $H_{cd}^{(0)}$. Alternative eliminations of $\sigma_y$ are discussed next.

**Z-axis rotation.**—Starting from the SP dynamical equation with $H_0 + H_{cd}^{(0)}$ that we write now in the form
\begin{equation}
\tag{10}
H_0 + H_{cd}^{(0)} = \begin{pmatrix}
Z_0 & P e^{-i\phi} \\
P e^{i\phi} & -Z_0
\end{pmatrix},
\end{equation}
where $\phi = \arctan(h \dot{\Theta}_0/2X_0)$, $0 \leq \phi < 2\pi$, and $P = [X_0^2 + (h \dot{\Theta}_0/2)^2]^{1/2}$, we may apply the transformation
\begin{equation}
\tag{11}
U_z = \begin{pmatrix}
e^{-i\phi/2} & 0 \\
0 & e^{i\phi/2}
\end{pmatrix},
\end{equation}
which amounts to a rotation about the $Z$ axis by $\phi$. Notice that because $U_z$ is diagonal in the bare basis, the bare-state populations do not change from the SP to the IP. In the corresponding IP, and with $K_z = \hbar U_z U_z^\dagger$, the interaction Hamiltonian becomes
\begin{equation}
\tag{12}
U_z^\dagger (H_0 + H_{cd}^{(0)} - K_z) U_z = \begin{pmatrix}
Z_0 - \hbar \omega/2 & P \\
P & -Z_0 + \hbar \omega/2
\end{pmatrix},
\end{equation}
without $Y \sigma_y$ component. It can be realized directly in the laboratory and we may treat it as well as a SP Hamiltonian linked to the $I'$ Hamiltonian $A_{1t}^0 H_0 A_0$, a common IP node for the two SP Hamiltonians in Eqs. (10) and (12), connected via $A_0$ and $U_z^\dagger A_0$ respectively. This Hamiltonian trio and the corresponding dynamical equations constitute a neat example of the dual physical frame scheme of Fig. 1(b). Eq. (12) provides an alternative shortcut path, that guarantees the same bare-state populations than $H_0 + H_{cd}^{(0)}$, and indeed it has been implemented experimentally for a condensate on an accelerating lattice, to avoid the realization of a $\sigma_y$ term with a second optical lattice. The transition from Eq. (10) to (12) was justified based on properties specific to the optical lattice setting in [13]. In fact the elimination of $\sigma_y$ in the Hamiltonian can be done formally for any physical realization, and its usefulness will depend on the feasibility to implement the modified X and Z terms, demonstrated for a condensate on an accelerating lattice, but more involved for a two-level atom in an oscillating field, see below.

The approach based on a Z-rotation is compared in Figs. 2 and 3 with the one based on adding to $H_0$ the counterdiabatic term $H_{cd}^{(1)}$ with the LZ scheme for $H_0$ (i.e. a constant $X_0$ and a linear in time $Z_0$). Fig. 2 shows the Hamiltonian matrix elements and Fig. 3 the populations of $|1\rangle$. $H_0$ and the corresponding population are also shown as a reference. The process time is chosen to be short so that adiabaticity and population inverion fail for this Hamiltonian. Instead, the two shortcuts lead to perfect population inversion. Their Z components are similar, but the X components have a rather different structure. A possible advantage of the superadiabatic+counterdiabatic approach using $H_0 + H_{cd}^{(1)}$ is the smaller value of the $X$-maximum, which reduces amplitude noise and the field intensity.

**Two-level atoms.**—In quantum optics, Eq. (3), with $X_0 = \hbar \Omega R/2$, $Y_0 = 0$, and $Z_0 = -\hbar \Delta/2$, represents a rotating frame IP Hamiltonian for a two-level atom in an oscillating field with angular frequency $\omega(t) = \omega_0 - \Delta(t)$, where $\omega_0$ is the (angular) transition frequency, $\Omega_R$ the (on-resonance) Rabi frequency and $\Delta$ the detuning, after having applied the electric dipole and rotating wave approximations (RWA).

For $K = K_L = -[\hbar \omega(t)/2] \sigma_z$ and $U = U_L = \exp[-(i/\hbar) \int_0^t K_L(t') dt']$ (As $U_L$ is diagonal in the bare basis, the populations are the same in interaction and
FIG. 2: (color online). \( Z \) and \( X \) Hamiltonian components for \( H_0 \) (dashed lines); \( z \) axis rotation Hamiltonian \( U_z^{(1)}(H_0 + H_{cd}^{(0)})U_z \) (thick blue solid lines); superadiabatic-counterdiabatic method Hamiltonian \( H_0 + H_{cd}^{(1)} \) (thin red solid line). \( \theta_0(t) = \alpha(t - T/2) \), and \( \alpha = -10, T = 20/|\alpha| \), in units \( \hbar = 1, \hbar_0 = 1 \).

FIG. 3: (color online). Populations of the bare state \( |1\rangle \) corresponding to the Hamiltonians depicted in Fig. 2. Same line codes as in that figure. Time in units of \( T/2 \).

Schrödinger pictures.) the corresponding \( S \) (RWA) Hamiltonian is

\[
K_L + U_L H_0 U_L^\dagger = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & \Omega R e^{i\theta} \\ \Omega R e^{-i\theta} & \omega_0 \end{pmatrix},
\]

where \( \theta(t) = \int_0^t \omega(t') dt' \). We can read from it the time dependent intensity, proportional to \( \Omega_R^2 \), the frequency of the field that has to be applied, \( \dot{\theta}/(2\pi) \), and the atomic transition frequency \( \omega_0/(2\pi) \). If we start instead with \( H_0 + H_{cd}^{(0)} \) in the IP DE and apply the same transformation as before, we get the SP Hamiltonian

\[
K_L + U_L (H_0 + H_{cd}^{(0)}) U_L^\dagger = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & \Omega_R e^{i\theta} \\ \Omega_R e^{-i\theta} & \omega_0 \end{pmatrix}.
\]

which requires in principle two fields dephased by \( \pi/2 \) sharing a common time-dependent frequency but with different time-dependent intensities \( \bar{A} \). A \( Z \)-rotation may also be applied but realizing the result is now complicated due to the time-dependence of the diagonal components. i.e. of the transition frequency. In this physical context that dependence would imply time dependent level-shift engineering with an additional laser. It is thus advisable to find alternative, simpler realizations of the shortcuts.

\[
H_0 + H_{cd}^{(0)}
\]

is not the only Hamiltonian that drives the populations along the ones of the adiabatic approximation for \( H_0 \). There is a whole family of them using different phases for the adiabatic base states, the simplest one being \( H_{cd}^{(0)} \) itself \[16, 18\]. Note that \( A_0^2(H_{cd}^{(0)} - K_0) A_0 = 0 \) so the state does not move at all in the corresponding IP, whereas in the DE driven by \( H_{cd}^{(0)} \) the populations will follow the ones for the adiabatic dynamics of \( H_0 \). By contrast, \( H_{cd}^{(1)} \) alone is not enough to take the system along the superadiabatic path defined by \( H_1 \). We could still get rid of \( H_0 \) and use as a shortcut to superadiabaticity \( H_{cd}^{(0)} := H_{cd}^{(0)} + H_{cd}^{(1)} \). To see why, use \( U_{01} = A_0 A_1 \), and notice that \( U_{01}(H_{cd}^{(0)} - i\hbar U_{01}(H_{cd}^{(0)} - U_{01} = 0 \). In any case \( H_{cd}^{(0)} \) is not so interesting for the present application as it combines the three Cartesian components.

Let us now take \( H_{cd}^{(0)} = K_0 \) as the reference IP Hamiltonian and try to implement it with different physical fields as in Fig. 1(b). Applying \( U_L \) we get the SP Hamiltonian

\[
H_S = K_L + U_L K_0 U_L^\dagger = \frac{\hbar}{2} \begin{pmatrix} -\omega_0(t) & -i\dot{\Theta}_0 e^{i\theta} \\ i\dot{\Theta}_0 e^{-i\theta} & \omega(t) \end{pmatrix},
\]

which is indeed problematic to realize because the atomic transition frequency should be time dependent. In other words, a simple IP Hamiltonian does not necessarily imply a simple experiment. To remedy this, keeping the same simple IP DE, we may use instead \( U' = e^{-(i/\hbar) \int_0^t K'(t') dt'} \), with \( K' = -(h/2)\omega_0 \pi \). This choice implies now a simple resonant interaction with constant frequency \( \omega_0 \) and \( \dot{S}' \) Hamiltonian

\[
H_{S'} = K' + U' K_0 U'^\dagger = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & -i\dot{\Theta}_0 e^{i\dot{\theta}} \\ i\dot{\Theta}_0 e^{-i\dot{\theta}} & \omega_0 \end{pmatrix}.
\]

Other single laser implementations may also be developed by starting instead with \( H_0 + H_{cd}^{(1)} \). The term \( H_{cd}^{(1)} \) modifies the detuning and Rabi frequency so that the transformation \( U_L \) would lead to an SP Hamiltonian with the same structure as Eq. \[16\], but with modified laser and Rabi frequencies. A further alternative to the superadiabatic iterations is the “invariants-based inverse engineering approach” \[18\].

Trap expansions.— The final example is a fast harmonic trap expansion, or compression, which is receiving much attention because of fundamental and practi-
The reference Hamiltonian is $H = p^2/(2m) + m \ddot{\omega} q^2/2$, where $\ddot{\omega} = \ddot{\omega}(t)$ is the time dependent angular frequency, $m$ is the particle mass, and $q$ and $p$ are position and momentum operators. The corresponding counterdiabatic term to avoid excitations is $H_{cd}^{(0)} = -(pq + qp)\ddot{\omega}/(4\ddot{\omega})$, whose direct laboratory implementation is problematic and was left as an open question. This difficulty is overcome by the transformation $U_q = \exp \left( i \frac{m \dddot{\omega}}{3 \dddot{\omega}} q^2 \right)$, which eliminates the cross terms; it produces from $H_S = H_a + H_{cd}^{(0)}$ the IP Hamiltonian $H_I = U_q^\dagger (H_S - i\hbar U_q U_q^\dagger) U_q = p^2/(2m) + m \ddot{\omega} q^2/2$, where

$$\ddot{\omega} = \left[ \ddot{\omega}^2 - \frac{3 \dddot{\omega}^2}{4 \dddot{\omega}} + \frac{\dddot{\omega}}{2 \dddot{\omega}} \right]^{1/2}.$$  

This Hamiltonian can actually be realized directly \[20, 21\] and considered in a different physical frame as an ordinary harmonic oscillator with modified frequency. To satisfy the scheme of Fig. 1(b) we may apply the scheme of Fig. 1(b) we may apply $H_{cd}^{(0)}$ to $H_a$ to $H_S$, where $H_I$ is identical. In fact, by imposing $\ddot{\omega}(t_f) = \ddot{\omega}(t_f) = 0$, the final state is also equal for both dynamics, even in phase, and the final vibrational state populations coincide with those of a slow adiabatic process.

Discussion. — We have first proposed schemes for which different interaction and Schrödinger picture dynamical equations represent different physical processes and interactions. These schemes have been later combined and exemplified to produce better, realizable shortcuts to adiabaticity for population inversion protocols, and for expansions and compressions. Similar manipulations may be applied as well to facilitate or improve shortcuts to adiabaticity for other operations such as controlled atomic transport \[22, 29\]. In fact the idea of designing the pictures to generate alternative, easier to handle physics, is applicable to a plethora of quantum systems, in particular, in the realms of quantum simulations, quantum control, or quantum information, where developing techniques to externally drive the systems for specific goals is a central objective.

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