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Multiple Schrödinger Pictures and Dynamics in Shortcuts to Adiabaticity

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A Schrödinger equation may be unitarily transformed into dynamical equations in different interaction pictures which describe a common physical process, i.e., the same underlying interactions 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 physical processes. 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.—In standard applications 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. The Schrödinger picture (SP) is often privileged as the primary description, representative of the physical or experimental setting, whereas the multiple interaction pictures (IPs) 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 (DEs) for the 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.

In sharp contrast to this standard application of the interaction picture just described, we propose in this Letter alternative relations such as the ones in Figs. 1(b) and 1(c) or more complex combinations, where the nodes may belong to different physical processes, as a way to design alternative and feasible experimental routes for operations that are *a priori* difficult or impossible to perform. We will thus 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]. Contrary to [1] which is devoted specifically to harmonic oscillator expansions, the schemes proposed here are more general and provide a unified treatment for internal and external degrees of freedom, complementary to existing approaches.

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, possible 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 trap expansions and transport of cold atoms without final excitation [6].

Multiple Schrödinger pictures.—To explain the multiframe schemes of Figs. 1(b) and 1(c) we shall review first some basic equations and notation. SP and IP states are related by a unitary transformation, $|\psi_I\rangle = U^\dagger|\psi_S\rangle$, $|\psi_S\rangle = U|\psi_I\rangle$, and evolve according to $i\hbar\partial_t|\psi_S\rangle = H|\psi_S\rangle$, $i\hbar\partial_t|\psi_I\rangle = H_I|\psi_I\rangle$, where H is the Hamiltonian in the SP and $H_I = U^\dagger(H - K)U$, with $K = i\hbar\dot{U}U^\dagger$, the corresponding IP Hamiltonian. H, H_I, and K may be generally time dependent. Note that when $U(t) = 1$ at initial and final times the states are equal in both pictures at those times. If, in addition, $\dot{U} = 0$ at boundary times, the Hamiltonians coincide there also. 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; i.e., in this case S and S' correspond to different physical realities. 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

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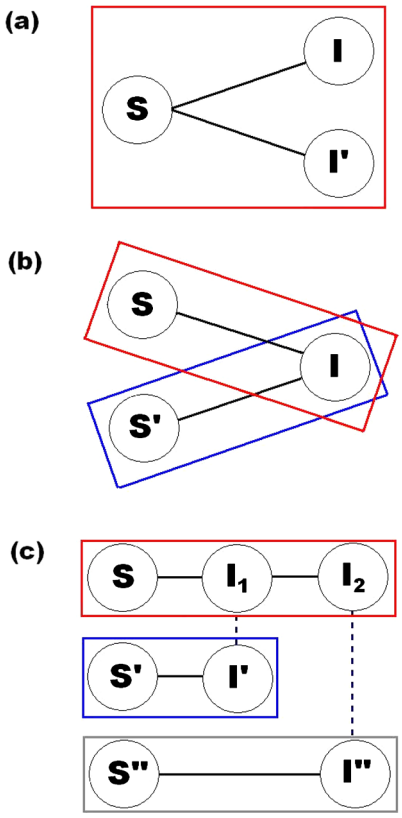


FIG. 1 (color online). Schematic relation between different Schrödinger and interaction picture dynamical equations. Each node may also represent the Hamiltonians or the states. The rectangular boxes enclose nodes that represent the same underlying processes. The solid lines connecting the nodes are unitary relations for the linked states, and the dashed lines represent a nonunitary addition of a term to the Hamiltonian.

several interpretations depending on the treatment given to the observables: If the observables are transformed, from B_S in S to $B_{S'} = U'U^\dagger B_S U U'^\dagger$ 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 $U^\dagger B_S U$ or $U'^\dagger B_S U'$, sharing in any case a common IP-state dynamics.

Another 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). Thus the nodes I' and I'' represent different physical processes (middle and lower horizontal boxes) with corresponding Schrödinger dynamics.

Superadiabatic iterations and counterdiabatic corrections.—In the following example the consecutive IPs of Fig. 1(c) are generated by means of adiabatic and superadiabatic iterations [7,8], and the addition of a "counterdiabatic" term in the Hamiltonian is performed so as to avoid transitions, canceling out the K [9]. This enables us to accelerate slow processes without inducing any final excitation. Our starting model Hamiltonian is

$$H_j(t) = \begin{pmatrix} Z_j(t) & X_j(t) - iY_j(t) \\ X_j(t) + iY_j(t) & -Z_j(t) \end{pmatrix}, \qquad (1)$$

i.e., $H_j = X_j\sigma_x + Y_j\sigma_y + Z_j\sigma_z$ in terms of Pauli matrices. (The index j will be used later to define a series of IP Hamiltonians in successive iterations). The Hamiltonian matrices are expressed in the "bare basis" of the two-level system, $|1\rangle = \binom{1}{0}$, $|2\rangle = \binom{0}{1}$. It could represent several physical systems such as a spin in a magnetic field, a two-level atom (see below), or a condensate in the bands of an accelerated optical lattice [10,11]. In the later case, X_j may be controlled by the trap depth, Z_j by the lattice acceleration [10], and a Y_j component could in principle be implemented by a second shifted lattice [11]. The Hamiltonian evolution or "trajectory" is specified here 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.

Let $j = 0$ and $Y_0 = 0$. 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, 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 $\{|n_0(t)\rangle\}$ that diagonalizes $H_0(t)$. Specifically we use $U = A_0(t) = \sum_{n=1,2}|n_0(t)\rangle\langle n_0(0)|$, where we assume that the $|n_0(0)\rangle$ coincide with the bare basis. Thus $|\psi_{I_1}\rangle = A_0^\dagger|\psi_S\rangle$ and $H_1 = A_0^\dagger(H_0 - K_0)A_0$, where $K_0 = i\hbar\dot{A}_0A_0^\dagger$. The phases are chosen so that $\langle n_0(t)|\dot{n}_0(t)\rangle = 0$. This makes K_0 nondiagonal and minimizes its norm [9,13]. In terms of the polar angle Θ_0, $K_0 = \hbar(\dot{\Theta}_0/2)\sigma_y$. The adiabatic approximation neglects K_0 in the IP Hamiltonian H_1 to trivially solve

$$i\hbar\partial_t|\psi_{I_1}\rangle = A_0^\dagger H_0 A_0|\psi_{I_1}\rangle, \qquad (2)$$

an uncoupled system in the bare basis. Alternatively one may add $A_0^\dagger K_0 A_0$ to H_1 [5,9,14–16]. The effect is to cancel any coupling so that Eq. (2) 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 $H_1 = A_0^\dagger(H_0 - K_0)A_0$ in the form of Eq. (1), $j = 1$, and diagonalize it to produce a "superadiabatic" basis $\{|n_1(t)\rangle\}$, and the transformation $A_1 = \sum_{n=1,2}|n_1(t)\rangle\times\langle n_1(0)|$. As before we assume that this basis coincides at

the boundary times with the bare basis and that $K_1 = i\hbar\dot{A}_1 A_1^\dagger$ is nondiagonal in $\{|n_1(t)\rangle\}$. A_1 produces a new IP [I_2 in Fig. 1(c)] with $|\psi_{I_2}\rangle = A_1^\dagger|\psi_{I_1}\rangle$, and Hamiltonian $H_2 = A_1^\dagger(H_1 - K_1)A_1$. K_1 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 $H_{cd}^{(1)} = A_0 K_1 A_0^\dagger$ [9]. 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, $H_{cd}^{(1)} = \hbar(\dot{\Theta}_1/2)(\cos\Theta_0\sigma_x - \sin\Theta_0\sigma_z)$, if $\dot{\Theta}_0 < 0$. The absence of a $Y\sigma_y$ component, like in H_0 and unlike in $H_{cd}^{(0)}$, 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 [11]. One more advantage of the superadiabatic shortcut is that $H_{cd}^{(1)}$ is less intense (it has a smaller norm) than $H_{cd}^{(0)}$ [9]. Alternative eliminations of σ_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

$$H_0 + H_{cd}^{(0)} = \begin{pmatrix} Z_0 & Pe^{-i\phi} \\ Pe^{i\phi} & -Z_0 \end{pmatrix}, \tag{3}$$

where $\phi = \arctan(\hbar\dot{\Theta}_0/2X_0)$, $0 \le \phi < 2\pi$, and $P = [X_0^2 + (\hbar\dot{\Theta}_0/2)^2]^{1/2}$, we may apply the transformation [17]

$$U_z = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix},$$

which amounts to a rotation about the Z axis by ϕ. Notice that because U_z is diagonal in the bare basis, the bare-state populations are the same in the SP and the IP at all times. In the corresponding IP, and with $K_z = i\hbar\dot{U}_z U_z^\dagger$, the interaction Hamiltonian becomes

$$U_z^\dagger(H_0 + H_{cd}^{(0)} - K_z)U_z = \begin{pmatrix} Z_0 - \hbar\dot{\phi}/2 & P \\ P & -Z_0 + \hbar\dot{\phi}/2 \end{pmatrix}, \tag{4}$$

without $Y\sigma_y$ component. It can be realized directly in the laboratory (this goes beyond the formal application in [17]) and we may treat it as well as a SP Hamiltonian linked to the I' Hamiltonian $A_0^\dagger H_0 A_0$, a common IP node for the two SP Hamiltonians in Eqs. (3) and (4), 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 scheme of Fig. 1(b). Equation (4) provides an alternative shortcut path, that guarantees the same bare-state populations as $H_0 + H_{cd}^{(0)}$, and indeed it has been implemented experimentally for a condensate on an accelerating lattice [11], to avoid the realization of a σ_y term with a second optical lattice. The transition from Eq. (3) to (4) was justified based on properties specific to the optical lattice setting in [11]. In fact the elimination of σ_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 [11], but more involved for a two-level atom in an oscillating field, see below.

The approach based on a Z rotation is compared in Fig. 2 with the one based on adding to H_0 the counterdiabatic term $H_{cd}^{(1)}$ with the Landau-Zener scheme for H_0 (i.e., a constant X_0 and a linear in time Z_0). The process time is chosen to be short so that adiabaticity and population inversion fail for the Hamiltonian H_0 alone while these two approaches lead to perfect population inversion. In Fig. 2, it can be seen that 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. (1), 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 ω_0 is the (angular) transition frequency, Ω_R the (on-resonance) Rabi frequency and Δ the detuning, after having applied the electric dipole and rotating wave approximations (RWAs). For $K = K_L = -[\hbar\omega(t)/2]\sigma_z$ and $U = U_L = \exp[-(i/\hbar)\int_0^t K_L(t')dt']$ the corresponding S (RWA) Hamiltonian is

$$K_L + U_L H_0 U_L^\dagger = \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & \Omega_R e^{i\theta} \\ \Omega_R e^{-i\theta} & \omega_0 \end{pmatrix}, \tag{5}$$

where $\theta(t) = \int_0^t \omega(t')dt'$. We can read from it the time-dependent intensity, proportional to Ω_R^2, the frequency of

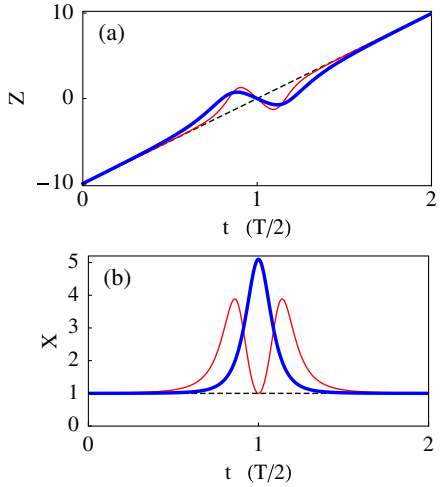


FIG. 2 (color online). Z and X Hamiltonian components for: H_0 (dashed lines); z-axis rotation Hamiltonian (4) (thick blue solid lines); superadiabatic + counterdiabatic method Hamiltonian $H_0 + H_{cd}^{(1)}$ (thin red solid lines). $Z_0(t) = -\alpha(t - T/2)$, and $\alpha = -10$, $T = 20/|\alpha|$, in units $\hbar = 1$, $X_0 = 1$.

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

$$K_L + U_L(H_0 + H_{cd}^{(0)})U_L^\dagger = \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & (\Omega_R - i\dot{\Theta}_0)e^{i\theta} \\ (\Omega_R + i\dot{\Theta}_0)e^{-i\theta} & \omega_0 \end{pmatrix},$$

which requires in principle two fields dephased by $\pi/2$ sharing a common time-dependent frequency but with different time-dependent intensities [5]. A Z rotation may also be applied but realizing the result is now complicated due to the time dependence of the diagonal components, this 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 $A_0^\dagger(H_{cd}^{(0)} - K_0)A_0 = 0$ 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 $H_{cd}^{(01)} :== H_{cd}^{(0)} + H_{cd}^{(1)}$, but 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

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

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 $K' = -(\hbar/2)\omega_0\sigma_z$. This choice implies now a simple resonant interaction with constant frequency ω_0 and S' Hamiltonian

$$H_{S'} = K' + U' K_0 U'^\dagger = \frac{\hbar}{2}\begin{pmatrix} -\omega_0 & -i\dot{\Theta}_0 e^{i\omega_0 t} \\ i\dot{\Theta}_0 e^{-i\omega_0 t} & \omega_0 \end{pmatrix}.$$

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 a SP Hamiltonian with the same structure as Eq. (5), but with modified laser and Rabi frequencies. An alternative to the superadiabatic iterations is the "invariants-based inverse engineering approach" [18].

Trap expansions.—A further example is a fast harmonic trap expansion, or compression, which is receiving much attention because of fundamental and practical implications [1,19–26]. The reference Hamiltonian is $H_h = p^2/(2m) + m\tilde{\omega}^2 q^2/2$, where $\tilde{\omega} = \tilde{\omega}(t)$ is the time-dependent angular frequency, m the particle mass, and q and p are position and momentum operators. The corresponding counterdiabatic term to avoid excitations is $H_{cd}^{(0)} = -(pq + qp)\dot{\tilde{\omega}}/(4\tilde{\omega})$, whose direct laboratory implementation is problematic and was left as an open question [6]. This difficulty is overcome by the transformation $U_q = \exp(i\frac{m\dot{\tilde{\omega}}}{4\hbar\tilde{\omega}}q^2)$, which eliminates the cross terms; it produces from $H_S = H_h + H_{cd}^{(0)}$ the IP Hamiltonian $H_I = U_q^\dagger(H_S - i\hbar\dot{U}_q U_q^\dagger)U_q = p^2/(2m) + m\tilde{\omega}'^2 q^2/2$, where $\tilde{\omega}' = [\tilde{\omega}^2 - \frac{3\dot{\tilde{\omega}}^2}{4\tilde{\omega}^2} + \frac{\ddot{\tilde{\omega}}}{2\tilde{\omega}}]^{1/2}$. This Hamiltonian can actually be realized directly [20,21] and considered in a different physical setting as an ordinary harmonic oscillator with modified frequency. (This is different from applying the transformation just to solve formally the dynamics with H_S, see e.g., [27].) To satisfy the scheme of Fig. 1(b) we may apply $U' = \mathbb{1}$ and regard H_I as a Schrödinger Hamiltonian S', namely $H_I = H_{S'}$. It indeed provides a shortcut with the following properties: Starting with a common state at time $t = 0$, the spatial densities driven by $H_h + H_{cd}^{(0)}$ and $H_{S'}$ are identical. In fact, by imposing $\dot{\tilde{\omega}}(t_f) = \ddot{\tilde{\omega}}(t_f) = 0$ 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.

Transport.—The final example is harmonic transport of a particle [28–31]. A Hamiltonian $H_0 = p^2/(2m) + [q - q_0(t)]^2 m\tilde{\omega}_0^2/2$, with $\tilde{\omega}_0$ constant, will generally induce excitations when moving the trap center $q_0(t)$. They are formally avoided by adding the counterdiabatic term $H_{cd}^{(0)} = p\dot{q}_0$ in $H_S = H_0 + H_{cd}^{(0)}$, which is, however, not realizable [30]. The transformation $U = e^{-im\dot{q}_0 q/\hbar}$ produces, after adding a time-dependent constant term, the feasible Hamiltonian $H_I = H_{S'} = p^2/(2m) + [q - q_0'(t)]^2 m\tilde{\omega}_0^2/2$, where $q_0' = q_0 + \ddot{q}_0/\tilde{\omega}_0^2$. In this and previous examples a Lie algebra of operators and the Baker-Haussdorff identity facilitate the elimination of physically undesirable terms.

Discussion.—We have first proposed schemes for which an interaction picture dynamical equation represents different physical processes and interactions. These schemes have been later combined and exemplified to produce better, realizable shortcuts to adiabaticity for population inversion protocols, for trap expansions and compressions, and for harmonic transport. Similar manipulations may be applied as well to facilitate or improve shortcuts to adiabaticity for other operations and may be extended to three-level applications [32,33]. 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 drive the systems for specific goals is a central objective.

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