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High-fidelity adiabatic passage by composite sequences of chirped pulses

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We present a method for optimization of the technique of adiabatic passage between two quantum states by composite sequences of frequency-chirped pulses with specific relative phases: composite adiabatic passage (CAP). By choosing the composite phases appropriately the nonadiabatic losses can be canceled to any desired order with sufficiently long sequences, regardless of the nonadiabatic coupling. The values of the composite phases are universal for they do not depend on the pulse shapes and the chirp. The accuracy of the CAP technique and its robustness against parameter variations make CAP suitable for high-fidelity quantum information processing.

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Introduction. Adiabatic passage (AP) techniques are a popular tool for coherent control of quantum systems due to their simplicity and insensitivity to variations in experimental parameters [1]. During adiabatic evolution, the system follows an eigenstate of the Hamiltonian — *adiabatic* (dressed) state. If the Hamiltonian is time-dependent this adiabatic state can be made to connect different *diabatic* (bare) states, and thereby produce population transfer. A variety of adiabatic techniques have been proposed and demonstrated, including rapid adiabatic passage [2], Stark-chirped rapid adiabatic passage [3], retroreflection-induced bichromatic adiabatic passage [4], superadiabatic passage [5], piecewise adiabatic passage [6], stimulated Raman adiabatic passage and its variations [7]. In rapid adiabatic passage, which is the oldest and simplest member of this family, the transition frequency of the two-state system and the carrier frequency of the driving external coherent field cross at some instant of time. A level crossing is created either by variation of the transition frequency (e.g. by Zeeman or Stark shifts) or by variation of the field frequency (e.g. by frequency chirping). This energy crossing, combined with adiabatic evolution, leads to population transfer between the two quantum states.

In nearly all AP techniques the population transfer is incomplete, with efficiency close to, but less than 1. In the traditional branches of quantum physics a fidelity of 90-95% usually suffices. However, in quantum information processing a much higher fidelity is needed, with an admissible error at most 10^{-4} [8]. Several methods for optimization of AP have been proposed, e.g., with fields that produce parallel eigenenergies [9], or additional fields that cancel the nonadiabatic coupling [10].

In this Letter, we propose a method for optimization of AP, which uses composite pulse sequences — composite adiabatic passage (CAP) — in which the single pulse driving the quantum transition is replaced by a sequence of pulses with well-defined relative phases. A suitable choice of these phases allows various imperfections in the inversion profile to be compensated to any desired order,

without even knowing the magnitude of the errors.

Composite pulses. Composite pulses, which generalize the concept of spin echo [11], have been invented in nuclear magnetic resonance (NMR) [12]. The available methods for construction of composite pulses use the intuitive notion of geometric rotations in the Bloch vector picture and they are applicable to pulses of rectangular temporal shape and constant detuning. Such shapes are adequate in NMR [12] and in atomic excitation with microsecond laser pulses [13], but cannot be used for pulses of smooth shapes and/or time-dependent detuning. Recently, an $SU(2)$ algebraic approach has been developed for the design of composite sequences of pulses with smooth temporal shapes and constant detuning [14]. Here we use this approach to construct composite pulses with *chirped* detuning, which allows us to optimize adiabatic passage through a level crossing.

A two-state quantum system driven by an external coherent field is described by the Schrödinger equation,

$$i\hbar\partial_t\mathbf{c}(t) = \mathbf{H}(t)\mathbf{c}(t), \quad (1)$$

where $\mathbf{c}(t) = [c_1(t), c_2(t)]^T$ is a vector-column with the probability amplitudes of the two states $|\psi_1\rangle$ and $|\psi_2\rangle$. The Hamiltonian after the rotating wave approximation [15] is $\mathbf{H}(t) = (\hbar/2)\Omega(t)e^{-iD(t)}|\psi_1\rangle\langle\psi_2| + \text{h.c.}$, with $D = \int_0^t \Delta(t')dt'$, where $\Delta = \omega_0 - \omega$ is the detuning between the field frequency ω and the Bohr transition frequency ω_0 , and $\Omega(t)$ is the Rabi frequency, which quantifies the field-system interaction. The evolution of the quantum system is described by the propagator \mathbf{U} , which connects the probability amplitudes at time t to their initial values at time t_i : $\mathbf{c}(t) = \mathbf{U}(t, t_i)\mathbf{c}(t_i)$. It is parameterized by the Cayley-Klein parameters a and b ,

$$\mathbf{U} = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix}. \quad (2)$$

The transition probability is $p = |b|^2 = 1 - |a|^2$. A constant phase shift ϕ in the driving field, $\Omega(t) \rightarrow \Omega(t)e^{i\phi}$,

is mapped onto the propagator as

$$\mathbf{U}_\phi = \begin{bmatrix} a & b e^{-i\phi} \\ -b^* e^{i\phi} & a^* \end{bmatrix}. \quad (3)$$

For experimental convenience, it is preferable to take all constituent pulses the same, with the same shape, width, peak Rabi frequency, detuning and chirp, and leave only their phases different. This restriction greatly simplifies the derivation; it is not, however, mandatory for the CAP technique. A composite sequence of N identical pulses, each with a phase ϕ_k , produces the overall propagator

$$\mathbf{U}^{(N)} = \mathbf{U}_{\phi_N} \mathbf{U}_{\phi_{N-1}} \cdots \mathbf{U}_{\phi_2} \mathbf{U}_{\phi_1}. \quad (4)$$

The composite phases ϕ_k ($k = 1, 2, \dots, N$) are control parameters, which are fixed by requiring a specific excitation profile. Because the overall phase does not affect the excitation profile, one of these phases can be set to zero. It is also convenient to have the ‘‘anagram’’ condition $\mathbf{H}_k(t) = \mathbf{H}_{N+1-k}(t)$ ($k = 1, 2, \dots, \lfloor N/2 \rfloor$), which leads to symmetric excitation profiles. For a composite sequence of $2n + 1$ pulses, we find $\phi_1 = \phi_{2n+1} = 0$ and we are left with n independent phases: $\phi_2 = \phi_{2n}$, $\phi_3 = \phi_{2n-1}$, \dots , $\phi_n = \phi_{n+2}$, and ϕ_{n+1} . We note that if a set of phases $\{\phi_k\}_{k=2}^{n+1}$ is a solution to the control problem then the set $\{-\phi_k\}_{k=2}^{n+1}$ is also a solution. All phases are determined with modulo 2π ; hence the set $\{2\pi - \phi_k\}_{k=2}^{n+1}$ is another solution.

Composite phases. We consider a model, in which the Rabi frequency $\Omega(t)$ is an even function of time and the detuning $\Delta(t)$ is odd,

$$\Omega(t) = \Omega(-t), \quad \Delta(t) = -\Delta(-t). \quad (5)$$

Then the Cayley-Klein parameter a in the propagator (2) is real, $a \in \mathbb{R}$ [16]. For a three-pulse sequence, with phases $(0, \phi, 0)$, we find from Eq. (4) that $U_{11}^{(3)} = a^3 - a|b|^2(1 + 2\cos\phi)$. The choice $\phi = 2\pi/3$ annuls the second term: $U_{11}^{(3)} = a^3$; then $U_{11}^{(3)}$ and its first two derivatives vanish at the point where $a = 0$, thereby making the excitation profile more robust to variations in the pulse area around this point. Because the dependence on ϕ factorizes in the second term of $U_{11}^{(3)}$, the composite phase $\phi = 2\pi/3$ does not depend on Ω and Δ . For a sequence of five pulses with phases $(0, \phi_2, \phi_3, \phi_2, 0)$, we find $U_{11}^{(5)} = a^5 - 2a^3|b|^2[1 + 2\cos\phi_2 + \cos(\phi_2 - \phi_3) + \cos\phi_3] + a|b|^4[1 + 2\cos(\phi_2 - \phi_3) + 2\cos(2\phi_2 - \phi_3)]$. Again, we can choose the phases ϕ_2 and ϕ_3 such that they nullify all but the first term: $U_{11}^{(5)} = a^5$. This corresponds to nullifying $U_{11}^{(5)}$ and its first four derivatives in the point where $a = 0$. One solution is $(\phi_2 = 4\pi/5, \phi_3 = 2\pi/5)$.

This idea can be generalized for pulse sequences, containing $N = 2n + 1$ pulses. In this case, choosing the phases appropriately, we have $U_{11}^{(N)} = a^N$, which leads

to transition probability $p = 1 - a^{2N}$. Since for the model (5) we have $a \in [-1, 1]$, then $p \rightarrow 1$ for $N \rightarrow \infty$, except for resonant even- π pulses, where $a = \pm 1$. In particular, for a sequence of N resonant ($\Delta = 0$) pulses, we obtain $p = 1 - \cos(A/2)^{2N}$, which tends to 1 for large N regardless of the pulse area A . We have derived a general analytic formula for the phases of a composite sequence of N pulses, which optimizes AP against variations in the pulse area and the chirp rate,

$$\phi_k^{(N)} = \left(N + 1 - 2 \left\lfloor \frac{k+1}{2} \right\rfloor \right) \left\lfloor \frac{k}{2} \right\rfloor \frac{\pi}{N}, \quad (6)$$

where $k = 1, 2, \dots, N$ and the symbol $\lfloor x \rfloor$ denotes the floor function (the integer part of x). These ‘‘magic’’ phases can be used to produce an arbitrarily accurate population inversion. The remarkable simplicity of the analytic expression (6) for the composite phases may have an underlying simple geometric interpretation.

Examples. The exactly soluble Demkov-Kunike (DK) model [17] assumes a sech pulse shape and a tanh frequency chirp added to a static detuning Δ_0 ,

$$\Omega(t) = \Omega_0 \operatorname{sech}(t/T), \quad \Delta(t) = \Delta_0 + B \tanh(t/T), \quad (7)$$

where Ω_0 , Δ_0 and B are constant parameters with the dimension of frequency, and T is the pulse width. For $\Delta_0 = 0$ (no static detuning) the DK model reduces to the Allen-Eberly (AE) model [18], which obeys the conditions (5), while for $B = 0$ (no chirp) it reduces to the Rosen-Zener model [19]. The Cayley-Klein parameter a in the DK model is expressed by Gamma functions,

$$a = \frac{\Gamma(\nu)\Gamma(\nu - \lambda - \mu)}{\Gamma(\nu - \lambda)\Gamma(\nu - \mu)}, \quad (8)$$

where $\lambda = \sqrt{\alpha^2 - \beta^2} - i\beta$, $\mu = -\sqrt{\alpha^2 - \beta^2} - i\beta$, and $\nu = \frac{1}{2} + i(\delta - \beta)$, with $\alpha = \Omega_0 T/2$, $\beta = BT/2$ and $\delta = \Delta_0 T/2$. The transition probability $p = 1 - |a|^2$ is

$$p = 1 - \frac{\cosh(2\pi\delta) + \cos(2\pi\sqrt{\alpha^2 - \beta^2})}{\cosh(2\pi\delta) + \cosh(2\pi\beta)}. \quad (9)$$

A transition probability $p = 1$ is obtained for $\delta = 0$ and $\sqrt{\alpha^2 - \beta^2} = n + \frac{1}{2}$, with $n = 0, 1, 2, \dots$. The transition probability tends to unity also in the adiabatic limit ($\alpha > |\beta| \gg 1$) for $\delta = 0$. However, if the chirp β is not large enough, nonadiabatic oscillations versus α appear and the probability is reduced. These oscillations can be suppressed to any order by composite pulses.

Figure 1 shows the dramatic improvement of adiabatic passage with composite pulses. Frames (a) and (b) show that a five-pulse CAP with sech-tanh shapes suffices to suppress the nonadiabatic oscillations below the quantum information benchmark 10^{-4} . Frames (c) and (d) show the optimization of AP for the experimentally more common situation of a Gaussian pulse with linear chirp, for which only an approximate analytic solution is known

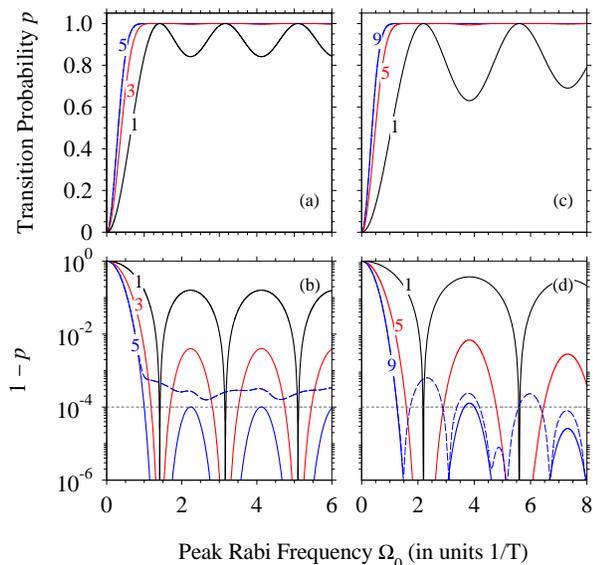


FIG. 1: Transition probability vs. peak Rabi frequency for a single pulse, and for N -pulse composite sequences (with N denoted on the curves) with phases from Eq. (6), assuming (a) sech-tanh pulses for chirp rate $B = 1/T$; (c) Gaussian pulses, $\Omega(t) = \Omega_0 e^{-t^2/T^2}$, with a linear chirp, $\Delta(t) = Ct$, with $C = 2/T^2$. Frames (b) and (d) show the infidelities of the respective upper profiles. The dashed curve in frame (b) is for pulse areas with a random error of 1% in the five-pulse sequence. The dashed curve in frame (d) is for an asymmetric pulse shape, $\Omega(t) = \Omega_0 e^{-t^2/T^2} [1 + \tanh(t/T)/20]$.

[20]; because conditions (5) are satisfied the composite phases are given by Eq. (6). The reduction of the nonadiabatic losses is not as high as for sech pulses because Gaussian pulses are less adiabatic [20]; however, the 10^{-4} error benchmark can still be reached, albeit with longer sequences. We point out that the composite phases (6) are applicable to other pulse shapes and chirps with the symmetry property (5), e.g. the Landau-Zener model [21] in its finite version [22].

We note that the compensation of nonadiabatic losses does not occur merely due to increased overall pulse area of the composite sequence. For example, the fidelity of the five-pulse CAP in Fig. 1 cannot be obtained with a single sech-tanh pulse with a five times larger area. Moreover, in an experiment it is often preferable, and more feasible, to use a sequence of pulses with a smaller area rather than a single pulse with a large area.

Another experimental issue are the conditions for equal pulse areas and symmetric pulse shapes. We include in Fig. 1(b) a curve with a 1% random error in the individual pulse areas; the infidelity remains close to the 10^{-4} benchmark. We further show in Fig. 1(d) a curve for asymmetric pulse shapes; we see that a small (5%) asymmetry does not affect the CAP technique significantly. For larger asymmetry the composite phases can always be calculated numerically; they may differ from the ones

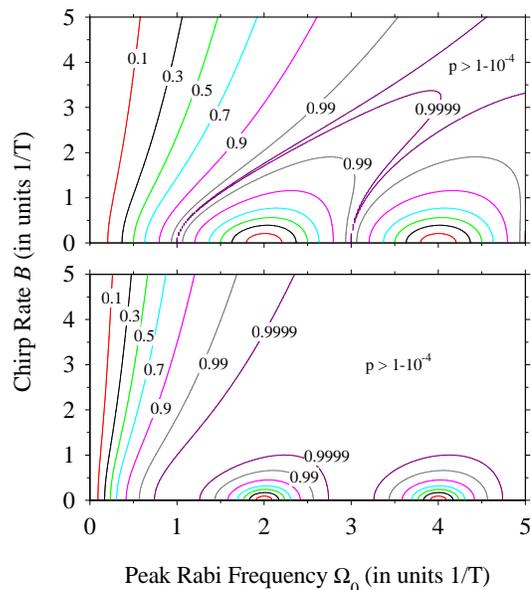


FIG. 2: Transition probability vs. peak Rabi frequency and chirp rate for a single AE pulse (top) and for a five-pulse composite sequence with phases $(0, 4\pi/5, 2\pi/5, 4\pi/5, 0)$ (bottom).

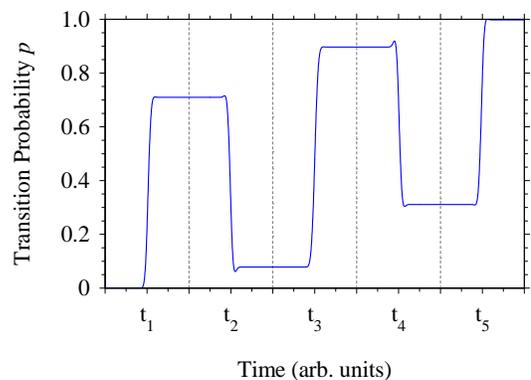


FIG. 3: Transition probability vs. time for a sequence of five pulses with Gaussian pulse shape, $\Omega_n(t) = \Omega_0 e^{-(t-t_n)^2/T^2}$, and linear chirp, $\Delta(t) = Ct$, with $\Omega_0 = 1.2/T$ and $C = 1/T^2$.

prescribed by us for symmetric pulses but the respective sequences should perform equally well.

The fidelity of the CAP technique is further illustrated in Fig. 2 versus Ω_0 and the chirp rate B . CAP greatly enhances the robustness of the transition probability against variations of Ω_0 and B and achieves ultra-high fidelity even for moderate parameter values and small number of constituent pulses.

The CAP technique must not be confused with the technique of piecewise adiabatic passage (PAP) [6], which also uses a sequence of phased pulses. PAP requires a large number of pulses, each of which produces a perturbatively small change in the populations, whereas CAP works for an arbitrary number of pulses and each pulse produces a large population change. Moreover, PAP de-

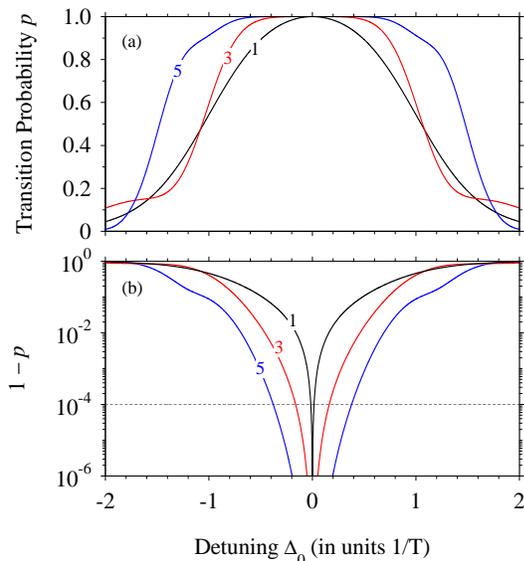


FIG. 4: (a) Transition probability vs. static detuning Δ_0 for a single sech-tanh pulse, Eq. (7), three- and five-pulse sequences with phases $(0, \pi/3, 0)$ and $(0, \pi/6, 5\pi/3, \pi/6, 0)$, respectively. The chirp rate is $B = 1/T$ and $\Omega_0 = \sqrt{2}/T$. (b) Infidelity of the profiles from frame (a).

mands phases that change quadratically from pulse to pulse, which translate into a linear chirp for a large number of pulses; the population evolution is a piecewise version of the one for standard single-pulse AP. In CAP the composite phases are derived from the condition to cancel the deviations from unit transfer efficiency due to nonadiabatic effects by enforcing destructive interference of these deviations. Figure 3 shows an example of population evolution during CAP, in which each constituent pulse produces a large population change but not complete inversion; the destructive interference of the deviations drives the system to complete inversion in the end.

Hitherto we have used the CAP technique to stabilize the transfer efficiency against variations in the pulse area and the chirp rate. The CAP technique can also optimize the excitation with respect to the static detuning Δ_0 . To this end, we take the expansion of the propagator versus Δ_0 around the point $\Delta_0 = 0$ and choose again the composite phases such that the first few derivatives of $U_{11}^{(N)}$ vanish. Figure 4 illustrates the stabilization of the transition probability versus Δ_0 achieved with composite sequences of three and five pulses. The width of the high-fidelity range, with an error below the 10^{-4} benchmark, increases from $0.02/T$ for a single pulse to $0.32/T$ for three pulses and $0.75/T$ for five pulses.

Conclusions. The proposed CAP technique is a simple and efficient method for optimization of adiabatic passage by using composite pulse sequences. It allows one to suppress the nonadiabatic oscillations in the transition probability and to reduce the error below the 10^{-4} quantum computation benchmark, even with simple three-

and five-pulse composite sequences. It is particularly important that the composite phases do not depend on the specific pulse shape and chirp as long as the latter satisfy the symmetry property (5). These features make the CAP technique a potentially important tool for ultrahigh-fidelity quantum information processing.

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