Steering an Eigenstate to a Destination

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The control of time evolution of a quantum state under various physical constraints is investigated and solved in the context of a two-level system. We have discovered a general scheme of steering an eigenenergy state to a destination without net nonadiabatic transitions, and we discuss how the result may be tested and utilized in practice.

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Precision measurements and applications in quantum mechanics often depend on the careful preparation and controlled evolution of a quantum state [1]. A commonly used means of coherent control is through the application of precisely tailored ac pulses [2], and there is also a large body of theoretical literature for optimal control of quantum states [3]. Adiabatic following is in principle another general method of coherent control [4], which has been used recently to prepare ultracold atoms in a particular Bloch band [5]. This method depends crucially on the slowness of time evolution of the Hamiltonian and can suffer some losses due to nonadiabatic transitions [6].

In this Letter, we show how to achieve the goal of adiabatic switching of a state without any amount of nonadiabatic transitions: an initial eigenstate remains completely an eigenstate at the final time when the Hamiltonian finishes an evolution. For simplicity and also for wide applications [7,8], we choose to address the problem in the context of a two-level system or equivalently a spin-1/2 in a magnetic field. We show that the adiabatic switching can always be achieved even with the field constrained in a plane and that complete spin reversal can be obtained by Zener-like Hamiltonians where one field component sweeps from $-\infty$ to $+\infty$ while the others remain constant. We also discuss how our results may be applied in practice. We believe that the concept of eigenstate steering should not be confined to two-level systems, but we leave the generalization to three or more energy levels to a future publication.

Basic discussions.—We start with some general discussions on the basic aspects of the control problem for the two-level system to set up the scope and strategy of our approach. We will proceed with the method of inverse solution of the Schrödinger equation or the Heisenberg equation of motion, while adding various physical constraints on the Hamiltonian later. Previous studies with this method have been very fruitful, with the discovery of exact solutions of generalized rotating wave states [9] and evolution loops [10]. A closely related method is known as tracking [11].

The most general form of a two-level Hamiltonian can be written as [12]

$$H = -\frac{1}{2}\left(B_1\sigma_x + B_2\sigma_y + B_3\sigma_z + B_0\mathbf{1}\right), \qquad (1)$$

where $\mathbf{1}$ is the 2×2 unit matrix, the σ's are Pauli matrices, and the B's are real functions of time. The time evolution of the states is completely described by a time dependent unitary matrix U, and one can solve the Schrödinger equation inversely to find the Hamiltonian that generates such an evolution,

$$H = i\,\frac{dU}{dt}\,U^{-1}. \qquad (2)$$

The story seems to be finished in a single line. However, for many applications, the control of only a single state is of concern, and one may not even be interested in the overall phase of the state. These will leave some design freedom in the choice of the Hamiltonian, which can then be used to accommodate physical constraints of the apparatus or to achieve some optimization goals [13].

The two components of a state can generally be written as [12]

$$\psi_1 = \cos(\alpha/2)e^{-i\beta/2}e^{-i\gamma/2}, \qquad \psi_2 = \sin(\alpha/2)e^{+i\beta/2}e^{-i\gamma/2}, \qquad (3)$$

where α, β, and γ are three real functions of time. Physically, α and β are the polar and azimuthal angles of the mean spin vector (Bloch vector) [12]

$$\mathbf{r} = (\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle) = (\cos\beta\,\sin\alpha, \sin\beta\,\sin\alpha, \cos\alpha)\,, \qquad (4)$$

while γ is the overall phase. Clearly, the four parameters of the Hamiltonian are not going to be uniquely determined by the three parameters of the wave function. One can

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allow an arbitrary time dependent B_0, with the remaining parameters of the Hamiltonian given by

$$\begin{aligned} B_1 &= -[(\dot\gamma + B_0)\sin\alpha\cos\beta - \dot\alpha\sin\beta], \\ B_2 &= -[(\dot\gamma + B_0)\sin\alpha\sin\beta + \dot\alpha\cos\beta], \\ B_3 &= -[\dot\beta + (\dot\gamma + B_0)\cos\alpha]. \end{aligned} \tag{5}$$

The control of the spin angles (α, β) can be discussed with no reference to the overall phase γ and the scalar part of the Hamiltonian B_0. Using the Heisenberg equations of motion, one finds [12]

$$\dot{\mathbf{r}} = \mathbf{r} \times \mathbf{B}, \tag{6}$$

where $\mathbf{B} = (B_1, B_2, B_3)$ is the magnetic field (torque vector) and the equation is also known as the Bloch equation. An invariant of the equation of motion is the magnitude r of the mean spin, which is, in fact, equal to 1 for a pure state [14]. If one is interested in the simultaneous motion of two spin vectors (two states) driven by the same field, then the angle between the spins is also an invariant of the equation of motion. Such a rigid body rotation can be completely described by the three Euler angles, which should then determine the three field components completely [9]. Here, however, we are interested in the control of a single state, for which a general solution for $\mathbf{B}$ can be written as

$$\mathbf{B} = \dot{\mathbf{r}} \times \mathbf{r} + f\mathbf{r}, \tag{7}$$

which involves a time dependent free parameter f. What is the physical meaning of f? If one observes the motion of $\mathbf{r}$ in a frame which rotates with an angular velocity $\vec\Omega$, the effective field changes to $\mathbf{B}' = \mathbf{B} + \vec\Omega$ [15]. If the frame is chosen to be that spanned by the orthogonal axes $\mathbf{r}$, $\dot{\mathbf{r}}$, and $\mathbf{r} \times \dot{\mathbf{r}}$, the angular velocity is then $\vec\Omega = \mathbf{r} \times \dot{\mathbf{r}}$, and the effective field is given by $\mathbf{B}' = f\mathbf{r}$. In other words, in the frame comoving with the spin vector, the effective field is purely in the direction of the spin with a magnitude and sign given by f.

The solution of the field (7) with $f = 0$ then has the physical meaning that it represents a kind of field that can be simulated by inertial forces in a rotating frame of reference. What kind of constraint must such a field satisfy? Because both $\mathbf{B} = \dot{\mathbf{r}} \times \mathbf{r}$ and $\dot{\mathbf{B}} = \ddot{\mathbf{r}} \times \mathbf{r}$ are perpendicular to $\mathbf{r}$, the vector $\mathbf{B} \times \dot{\mathbf{B}}$ must be parallel to it. Therefore, if we calculate the time derivative of the unit vector of $\mathbf{B} \times \dot{\mathbf{B}}$, the result must have the same magnitude as $|\dot{\mathbf{r}}| = B$, i.e.,

$$\left|\frac{d}{dt}(\mathbf{n} \times \dot{\mathbf{n}}/|\dot{\mathbf{n}}|)\right| = B, \tag{8}$$

where $\mathbf{n}$ is the unit vector of $\mathbf{B}$. This condition can be made geometrically more transparent by writing it in the form

$$v\left|\mathbf{n} \times \frac{d^2\mathbf{n}}{ds^2}\right| = B, \tag{9}$$

where $v = |\dot{\mathbf{n}}|$ is the speed along the curve of $\mathbf{n}(t)$, and $s = \int dt\, v$ is the length variable of the curve. The above condition then means that the magnitude of the field B must be equal to the product of the speed and geodesic curvature of the curve formed by its directional unit vector.

Planar fields.—The free parameter f can be used to accommodate physical constraints in experiments. A highly interesting case in practice is that the field is restricted to a single plane [7,8]. Without losing generality, we take this plane to be the x-y plane. The condition of $B_3 = 0$ in Eq. (7) fixes the parameter $f = \dot\beta \sin\alpha \tan\alpha$. The other two components of the field are then fixed to be

$$\begin{aligned} B_1 &= \dot\alpha \sin\beta + \dot\beta \tan\alpha \cos\beta, \\ B_2 &= -\dot\alpha \cos\beta + \dot\beta \tan\alpha \sin\beta. \end{aligned} \tag{10}$$

These expressions are smooth everywhere except at the equator $\alpha = \pi/2$. Therefore, any spin motion that is localized entirely within the north or the south hemisphere can be generated by a field which lies completely on the equator plane. This result may have some implication on the issue of dynamical localization in a double well potential, which is often modeled as a two-level system (one level from each well) [16].

The spin motion under a finite planar field is necessarily restricted in the manner that $\dot\beta$ must vanish when it crosses the equator $\alpha = \pi/2$. This implies that if the spin crosses the equator at a finite rate ($\dot\alpha \neq 0$), the trajectory must be vertical at the equator ($\frac{d\alpha}{d\beta} = \frac{\dot\alpha}{\dot\beta} = \pm\infty$). However, if the spin approaches the equator with a vanishing rate, $\dot\alpha = 0$, the trajectory does not have to be vertical and can be even tangential to the equator. In any case, if one is interested only in achieving a target final state from a specific initial state, a planar field is more than sufficient. There is a general theorem [17] that almost any rotation of the states can be generated by the successive applications of two different components of the field, and our solution shows that the same can be achieved with smooth evolution of the field with two components. In the following, we wish to find solutions of the control problem that has additional requirements on the initial and final field directions.

Suppose the spin was initially fixed to a direction in which the field lies. Is it possible to bring the spin into another direction when the field rotates into that direction? According to the adiabatic theorem, this can be done up to exponentially small errors if the speed of field rotation is always much slower than its magnitude, which gives the separation between the energies of the two adiabatic eigenstates [4,6]. However, it is possible to devise solutions without any amount of nonadiabatic corrections and with the speed of field rotation not necessarily slow. To achieve this, one can simply specify a spin motion with $\dot{\mathbf{r}} = 0$ at the initial and final times and obtain the necessary time dependent field from the inverse solution in Eq. (7). This simple method does not work when there is a constraint on the field. For the case where the field lies on a plane, an exact solution was provided in Eqs. (4.49) of Ref. [7] with the desired property. Here we show a general method for obtaining such solutions, which requires that $\alpha \to \pi/2$, $\beta \to \theta$ at the initial and final times, where θ is the angle of the field with the x axis. To make these requirements more concise, we rewrite Eq. (10) in terms of the polar coordinates of the field as

$$B = (\dot{\alpha}^2 + \dot{\beta}^2 \tan^2\alpha)^{1/2}, \quad (11)$$

$$\theta = \beta - \tan^{-1}(\alpha' \cot\alpha), \quad (12)$$

where $\alpha' = \frac{d\alpha}{d\beta}$. The disappearance of time derivatives in Eq. (12) shows that the angle of the field is a geometric property of the trajectory, i.e., once α is known as a function of β, the angle θ is known as a function of β as well, regardless of how β may depend on time [18]. The condition of $\beta \to \theta$ can then be expressed as a geometrical condition of the trajectory, $\alpha' \cot\alpha \to 0$, as $\beta \to \theta_\mp$, where $\theta_\mp$ is the initial and final angles of the field. Therefore, if $|\alpha - \pi/2|$ goes to zero as $|\beta - \theta_\pm|^{p_\pm}$, the above condition is equivalent to $p_\pm > 1/2$. In the example given in Ref. [7], one effectively has a spin trajectory of the form $\sin\beta \tan\alpha = \text{const}$, corresponding to $\beta_\pm = 0,\ \pi$, and $p_\pm = 1$.

Zener-like models.—We now add one more physical constraint to our Hamiltonian: only one field component can vary in time. In the prototype adiabatic transition problem, the Zener problem [6], the parameters of the Hamiltonian may be written as $B_1 = \Delta$, $B_2 = vt$, and $B_3 = 0$. Then $\theta = \tan^{-1}(vt/\Delta)$, and the polar and azimuthal angles α, β can be expressed in terms of parabolic cylinder functions. If the initial spin lies in the field direction at $t = -\infty$, one finds that it will deviate from the field at $t = \infty$ by an angle given by $2\sin^{-1}[\exp(-\pi\Delta^2/2\hbar v)]$, which signifies a finite probability of nonadiabatic transitions. In contrast, we will show that it is possible to construct a similar Hamiltonian, but the net nonadiabatic excitation vanishes completely [19].

Our model Hamiltonian has the form with $B_3 = 0$, $B_1 = \text{const}$, and with B_2 changing monotonically from $-\infty$ to $+\infty$ in a manner similar to the Zener model. We wish to construct trajectories yielding $\alpha \to \pi/2$ and $\beta \to \pm\pi/2$ at the initial and final times, corresponding to a complete spin reversal with the field. These are satisfied, for instance, by the family of trajectories (Fig. 1) defined by $\sin\alpha = \exp[-\epsilon \cos^q\beta]$, with $\epsilon > 0$ and $q > 1$, where the latter inequality stems from the condition of $p_\pm > 1/2$ given earlier. The behavior of the field component B_2 is then fixed as follows. From the condition of $B_1 = B\cos\theta = \Delta$ and Eqs. (11) and (12), we find that

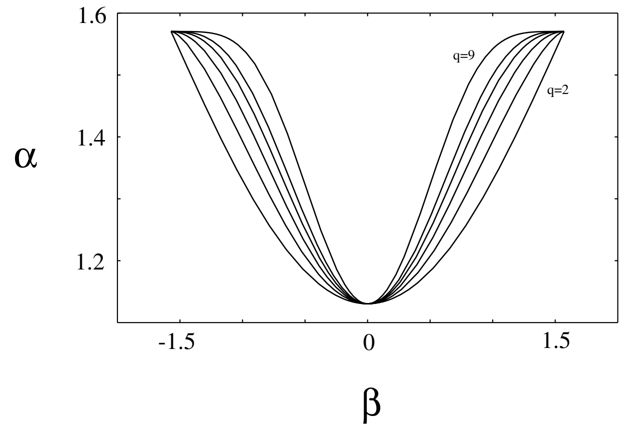

FIG. 1. A family of trajectories defined by $\sin\alpha = \exp[-\epsilon \cos^q \beta]$, shown with $\epsilon = 0.1$ and $q = 2, 3, 4, 5, 6, 9$, in increasing order from $q = 2$ to $q = 9$.

$$t\Delta = \int_0^\beta d\beta \sqrt{\alpha'^2 + \tan^2\alpha}\, \cos[\beta - \tan^{-1}(\alpha' \cot\alpha)], \quad (13)$$

where we have taken the zero of time to be at $\beta = 0$. Therefore, given a trajectory of the spin $\alpha = \alpha(\beta)$, the above equation fixes the dynamics (β as a function of time). This knowledge then determines the time dependence of B_2 completely:

$$B_2 = B\sin\theta$$
$$= \dot{\beta}\sqrt{\alpha'^2 + \tan^2\alpha}\, \sin[\beta - \tan^{-1}(\alpha' \cot\alpha)]. \quad (14)$$

Summarizing the arguments, all such time dependent fields will necessarily lock the spin to their directions at the initial and final times.

We now analyze the behavior of the field component B_2, using the above example of the spin trajectories (Fig. 2). For short times, we find that it goes through zero linearly as

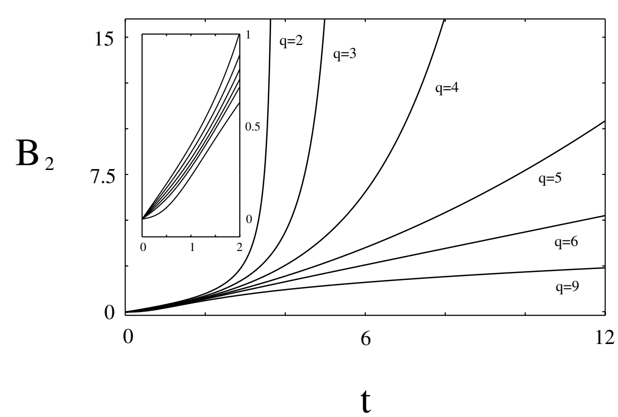

FIG. 2. Time dependence of B_2 for Zener-like models with $B_1 = 1$ that gives rise to the spin trajectories shown in Fig. 1. The inset shows the behavior at short times.

$B_2 = \Delta^2(1 - q\epsilon)\sqrt{e^{2\epsilon} - 1}\, t$, just like the Zener model. The behavior at large times depends on the value of q. For $q > 4$, it diverges as $\pm\Delta|(q/2 - 2)\sqrt{2\epsilon}\,\Delta t|^{\frac{2}{q-4}}$ as $t \to \pm\infty$. Therefore, one can achieve complete asymptotic spin locking by a field that diverges sublinearly, linearly, or superlinearly at large times. The linear divergence occurs at $q = 6$, but this does not mean that we have reduced to the Zener model, because the slopes at small and large times are different. Nevertheless, for $\epsilon \ll 1$, the slopes are almost the same, and our model may be regarded as an approximation to the Zener model but with no nonadiabatic transitions. In the marginal case of $q = 4$, we have the exponential divergence $B_2 \to \pm\Delta \exp[\Delta\sqrt{2\epsilon}\,|t|]$. For $1 < q < 4$, the asymptotic spin angles and the field values are reached at finite times as is signified by the convergence of the integral (13) at $\beta = \pm\pi/2$.

Applications.—Finally, we discuss possible applications of our findings. A basic operation in the field of quantum information is the rotation of a qubit [20], the transition from one quantum state to another or to a certain superposition of them, which is usually achieved by the application of a precisely tailored ac pulse. If the qubit is physically represented by a spin, then our method shows directly how it may be rotated as desired, with the additional benefit that it aligns with the field both at the initial and final times and is thus protected against small perturbations such as noise and dissipative processes at the beginning and the end of the operation. If the qubit is represented by a two-level atom, one needs to shine a laser chirping from well below to well above the resonant frequency in order to achieve our Zener-like model. In the rotating-wave frame of reference and within the rotating-wave approximation, this effectively reduces to our spin model with one component of the field given by the detuning and another given by the dipole coupling amplitude [7].

For another application, one may use our scheme to improve the design of optical lattice motion to accelerate cold atoms to high speed. The optical acceleration method has been used to prepare atoms to appropriate initial conditions and to observe a number of classic quantum effects in condensed matter physics [5]. For a constant acceleration, there is a finite probability for the atoms to tunnel out of a Bloch band. The tunneling is dominated by a gap of avoided crossing of two bands and can be effectively analyzed by the Zener model with B_1 given by the energy gap and with B_2 changing at a constant rate proportional to the acceleration. One should be able to shut off the tunneling completely by modifying the acceleration in time according to our design for $B_2(t)$. A detailed theoretical study of tunneling prohibition using an ac field has been undertaken in parallel by Catanzariti and Dunlap [21].

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