Stabilizing dynamical localization in driven tunneling

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(Received 18 June 1998)

Dynamical localization of a tunneling system by means of an oscillating external field is examined for an arbitrary doublet of tunneling states. We show that the condition of an exact crossing of Floquet levels, required for localization in a symmetric system, can be substantially relaxed for tunneling systems with broken symmetry. This generalization equally applies to tunneling systems coupled to a dissipative environment.

PACS numbers: 03.65.-w, 05.30.-d, 61.16.Ch, 62.65.+k

A tunneling particle can be localized indefinitely by an external periodic force. This surprising prediction was made recently by Grossmann et al. [1,2]. With properly chosen frequency and amplitude the external force can pin the tunneling particle, and the amplitude of the tunneling oscillations can be made arbitrarily small. Numerous methods have since been applied to study this effect, focusing on special cases which lend themselves to analytical solutions [3–8], or on their generalizations to tunneling systems with dissipation [9–16]. Previous works are based on the central assumption that an exact crossing of Floquet levels is necessary for dynamical localization to occur. For Floquet levels to cross, the tunneling system typically has to be symmetric, and the driving amplitude must be selected from a set of discrete “magic numbers”, different for each driving frequency [7].

In this Letter, we show that the tunneling particle can remain pinned even if both of the above conditions are relaxed simultaneously. This implies that the class of systems in which the dynamical localization can potentially be detected is much wider than previously thought. These include tunneling systems which are not intrinsically symmetric, such as tunneling of an atom between a sample and an STM tip [18], or tunneling in disordered systems like structural glasses [19,20]. We demonstrate that these findings also apply to dissipative tunneling systems, where the localization effect manifests itself through a suppression of tunneling oscillations and a drastic slowing down of the incoherent dynamics.

To study driven tunneling systems, we can either use a double-well potential model [1] or, more simply, a truncated two-state Hamiltonian [2]

$$H_0 = -\frac{\hbar \Delta}{2} \sigma_x - \frac{\hbar}{2} (\varepsilon_0 + \tilde{\varepsilon} \sin \omega t) \sigma_z. \quad (1)$$

This truncation is valid if all parameters are small compared to the lowest oscillation frequency $\omega_{\text{osc}}$ associated with the double well, and for a barrier height larger than $\hbar \omega_{\text{osc}}$. $\sigma_x$ and $\sigma_z$ are Pauli spin matrices, $\hbar \Delta$ is the tunnel splitting, $\hbar \varepsilon_0$ an intrinsic energy bias, and $\hbar \tilde{\varepsilon} \sin \omega t$ its modulation by an external periodic force.

Despite the simplicity of this Hamiltonian, its dynamics shows surprising effects in parameter regimes for which the rotating-wave approximation fails. A general analytical solution is not available, hence a detailed understanding of its dynamics must rely on numerics.

The Hamiltonian (1) is non-conservative, but it exhibits discrete time-translational invariance with period $T = 2\pi/\omega$. Consequently, the one-period time translation operator $U_T = U(T, 0)$ contains all essential information about the dynamics. Previous studies [1,2] concentrated on the case where two Floquet states, the eigenstates of $U_T$ in the two-state description, are degenerate. In that case, $U_T$ is the identity operator (or its negative), and the time dependence of all observables is strictly periodic with period $T$. Within the interval $T$, the population $p(t)$ of the initially occupied site exhibits small oscillations, with a minimum $p_{\min}$ such that $|1 - p_{\min}| \ll 1$.

In this work, we will consider this inequality the definition of localization and make no assumptions about the spectrum of $U_T$. In general, $p_{\min}$ is to be defined as the largest lower bound (infimum) of $p(t)$ for any positive $t$,

$$p_{\min} = \inf_{t \geq 0} p(t). \quad (2)$$

Although $t$ is unbounded, $p_{\min}$ can be evaluated without controlled approximations or extrapolation. Using the group properties of discrete time translations, the dynamics at arbitrary time $t$ can be constructed from the time translation operator at times $\tau \leq T$,

$$U_t = U_\tau U_T^n. \quad (3)$$

Here we have defined $U_\tau = U(t, 0)$, with $t = nT + \tau$, $0 \leq \tau < T$. The lower bound $p_{\min}$ is thus given by

$$p_{\min} = \min_{0 \leq \tau \leq T} \inf_{n \geq 0} p_n(\tau), \quad (4)$$

where

$$p_n(\tau) = |\langle \psi_0 | U_\tau U_T^n | \psi_0 \rangle|^2 \quad (5)$$

generally defines an infinite set of functions on the interval $0 \leq \tau \leq T$.

To obtain the infimum with respect to $n$, it is useful to represent the SU(2) matrix $U_T$ by a generator $g$ and an angle $\varphi_0$, $U_T = \exp(\frac{\tau}{2} \varphi_0 g)$. The unit vector $\vec{n}$ in $g = \vec{n} \cdot \vec{\sigma}$ denotes the rotation axis of the corresponding SO(3) rotation. Now $p_n$ reads

$$p_n(\tau) = |\langle \psi_0 | \exp\left(\frac{\tau}{2} \vec{n} \cdot \vec{\sigma} \varphi_0\right) | \psi_0 \rangle|^2, \quad (6)$$
and one can define a quantity closely related to \( p_n(\tau) \) with a continuous index \( \varphi \),

\[
\tilde{p}_\varphi(\tau) = |\langle \psi_0 | U_\tau \exp \left( \frac{\tau}{\hbar} \varphi \sigma \right) | \psi_0 \rangle|^2,
\]

where \( 0 \leq \varphi \leq 4\pi \). The set of functions \( \{ p_n(\tau) \} \) is a subset of \( \{ \tilde{p}_\varphi(\tau) \} \), i.e.,

\[
\min_{0 \leq \varphi \leq 4\pi} \tilde{p}_\varphi(\tau) \leq \inf_{n \geq 0} p_n(\tau).
\]

For generic parameters, \( \varphi_0/\pi \) is an irrational number. The set \( \{ \exp(\frac{\tau}{\hbar} \varphi_0 \sigma) \ | \ n \geq 0 \} \) is a dense subset of \( \{ \exp(\frac{\tau}{\hbar} \varphi \sigma) \ | \ 0 \leq \varphi \leq 4\pi \} \), and strict equality holds in (8). But in the degenerate case of rational \( \varphi_0/\pi \), the situation is different. \( p(\tau) \) is periodic, and there are only a finite number of functions \( p_n(\tau) \) that are distinct. We shall consider the latter case irrelevant in the long-time limit, because any minute drift or other aberration in the driving frequency or amplitude will reduce it to the generic case. We will concentrate on the generic case in the following.

For the two-state system, \( \tilde{p}_\varphi(\tau) \) is a continuous function of \( \varphi \) and \( \tau \), taking the form \( \tilde{p}_\varphi(\tau) = a_\tau + b_\tau \sin \varphi + c_\tau \cos \varphi \). The coefficients \( a_\tau \), \( b_\tau \), and \( c_\tau \) are algebraic functions of the matrix elements of \( U_\tau \) and \( U_{-\tau} \). From the numerical solution of the Schrödinger equation over a single period one can thus easily obtain the entire set of functions \( \tilde{p}_\varphi(\tau) \), and also the lower and upper envelopes of the set of curves \( p_n(\tau) \),

\[
p_{\text{le}}(\tau) = \inf_{n \geq 0} p_n(\tau) = \min_{0 \leq \varphi \leq 2\pi} \tilde{p}_\varphi(\tau),
\]

\[
p_{\text{ue}}(\tau) = \sup_{n \geq 0} p_n(\tau) = \max_{0 \leq \varphi \leq 2\pi} \tilde{p}_\varphi(\tau).
\]

According to (8), \( p_{\text{min}} \) is then given by the minimum of the lower envelope,

\[
p_{\text{min}} = \min_{0 \leq \tau \leq T} p_{\text{le}}(\tau).
\]

For a symmetric system driven at frequencies \( \omega \gg \Delta \), \( p_{\text{min}} \) has been shown to be almost unity if the ratio \( \dot{\varepsilon}/\omega \) belongs to a set of discrete ‘magic numbers’ for which \( U_\tau \) is diagonal and its eigenstates degenerate [2]. In the high-frequency limit, these numbers are the zeros \( z_n \) of the Bessel function \( J_0(z) \). But with even a slight deviation from these numbers, the degeneracy of the Floquet states will be lifted and \( U_\tau \) will have delocalized eigenstates, which manifest themselves as slow oscillations in \( p(\tau) \) with large amplitude and a reduced tunneling frequency \( \Delta J_0(\dot{\varepsilon}/\omega) \).

The central finding of this Letter is that the instability of the localization effect can be suppressed by imposing a small static bias \( \varepsilon_0 \) on the tunneling system. This is demonstrated by the numerical data in Fig. 1a. For a symmetric system (dashed curve), a slight detuning of the amplitude from its magic value leads to a slow coherent transition that depopulates the initial state. Adding a small bias, however, prevents this depopulation even out to very long times (solid curve). Fig. 1b shows the corresponding set of curves \( p_n(\tau) \) for \( 0 \leq n \leq 3 \) as well as the lower and upper envelopes \( p_{\text{le}}(\tau) \) and \( p_{\text{ue}}(\tau) \). This rigorous result for \( p_{\text{le}} \) shows unequivocally that a very robust localization persists indefinitely for the detuned system. The periodic function \( p(\tau) \) for the corresponding symmetric system with perfectly tuned amplitude \( \dot{\varepsilon}/\omega \approx 2.393 \) is given for comparison (dashed curve). Both cases show roughly equal \( p_{\text{min}} \).

How large does the bias need to be in order to effect dynamical localization, and is there a maximum allowable value for it? The precise answer depends quite sensitively on the driving parameters. We can look for the answer using the seminumerical procedure outlined above. The global minimum in Eq. (11) can easily be obtained by linear search because \( p_{\text{le}}(\tau) \) is smooth. Fig. 2 presents quantitative results about the dependence of \( p_{\text{min}} \) on \( \varepsilon_0 \) for different \( \dot{\varepsilon} \) in a tunneling system driven at \( \omega = 5\Delta \). The width of the minimum at \( \varepsilon_0 = 0 \) vanishes as \( \dot{\varepsilon}/\omega \) approaches the localization point of the symmetric system, i.e., the bias required to enable localization goes to zero. On the other hand, for very large bias \( \varepsilon_0 \approx \omega \), \( p_{\text{min}} \) drops drastically, and the dynamics is then characterized by large oscillations [3].

A qualitative understanding of this generalized localization effect is obtained by evaluating the dynamics at finite time analytically in the limit of high frequency [3]. For \( \omega \gg \max(\varepsilon_0, \Delta) \), we find \( |p_{\text{le}}| \ll 1 \), and \( g = N^{-1}(\Delta J_0(\dot{\varepsilon}/\omega) \sigma_x + \varepsilon_0 \sigma_z) \). From this we conclude that localization is possible if either (i) \( \varphi_0 = 0 \) (Floquet level crossing) or (ii) \( |J_0(\dot{\varepsilon}/\omega)| \ll |\varepsilon_0/\Delta| \) (axis \( \bar{n} \) aligned with the z axis). The two cases are closely related. In either case, driving modulates the transitions amplitudes giving rise to the off-diagonal elements of \( U_\tau \). In the first case, this is done in such a way that destructive interference makes the off-diagonal elements vanish precisely. In the second case, this cancellation is imperfect, but the residual off-diagonal elements are small enough to permit localized eigenstates of \( U_\tau \).

In a condensed matter environment, tunneling is coupled to fluctuations of the surrounding medium, and the delicate cancellations underlying this localization effect are disturbed by dissipation and dephasing. The standard approach to linear dissipation resulting from such a coupling generalizes the two-state system to the driven spin-boson Hamiltonian [2,22].

\[
H = H_0 + \sum_\nu \omega_\nu \left( a_\nu^\dagger a_\nu + \frac{1}{2} \right) + \frac{q_0}{2} \sum_\nu C_\nu (a_\nu + a_\nu^\dagger) \sigma_z.
\]

Here and in the following we set \( \hbar = 1 \); \( q_0 \) is the distance between tunneling sites. The effect of the harmonic environment is fully characterized by the spectral density \( J(\omega') = \pi \sum_\nu C_\nu^2 \delta(\omega' - \omega_\nu) \). Its specific form depends on the density of states of the dissipative environment and the details of their local interaction with the tunneling system. The Ohmic form \( J(\omega') = \eta \omega' \exp(-\omega'/\omega_c) \) is one of the most frequently investigated [2,22]. \( q_0 \) and \( \eta \) appear in the dynamics only through the dimensionless dissipation constant \( \alpha = \eta q_0^2 / 2\pi \).

In the case of large \( \omega_c \) applicable to tunneling in solid-state
systems, $\Delta$ and $\omega_c$ enter only through the scaled tunneling frequency $\Delta_r = \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$.

With the notable exception of the noninteracting-blip approximation (NIBA) [21,22] and certain limiting cases, the dynamics governed by the driven spin-boson Hamiltonian appears to be intractable without resorting, at least partially, to numerical methods. The recently introduced chromostochastic quantum dynamics (CSQD) algorithm [23] makes possible the exact and efficient computation of all dynamical quantities of interest in the spin-boson system. The CSQD method minimizes memory effects inherent to quantum dissipation by direct sampling of the colored noise produced by the environment. The statistical error increases only moderately with $t$; in the examples given below it never exceeds $7 \times 10^{-3}$.

The dynamics at low temperature and weak damping closely resembles that of the undamped system. Fig. 3 illustrates dynamical localization in a weakly damped asymmetric tunneling system with $\bar{\epsilon}/\omega = 2.3$ driven at $\omega = 5\Delta_r$. For a symmetric system, the same parameters result in a coherent population transfer between the two localized states. This transfer is strongly suppressed when a moderate bias $\epsilon_0 = -1$ is introduced. The system now exhibits a gradual population decay on a much longer timescale. Comparison with the free population decay of the biased system (without driving) shows that the bias $\epsilon_0$ alone is not sufficient to cause localization. In this example, the tunneling particle is actually localized on the site whose energy is raised by the bias. Fig. 4 shows the same driven system with $\epsilon_0 = -1$ (top) and $\epsilon_0 = 1$ (bottom) with little difference between the two curves, reminiscent of the symmetry seen in Fig. 2. The center plot shows a symmetric system driven at the same frequency, but with the amplitude needed for a Floquet crossing, $\bar{\epsilon}/\omega \approx 2.393$. Evidently, the two cases of localization discussed above lead to nearly identical behavior also in the dissipative case.

We have demonstrated that the remarkable effects resulting from dynamical localization in tunneling systems occur for a wide range of parameters that do not obey the restrictive conditions for an exact Floquet level crossing. We believe that these findings should stimulate further theoretical and experimental investigation. The prospect of an experimental realization has improved appreciably. The hard-to-satisfy requirements of an extremely precise control of the driving amplitude and its perfect homogeneity throughout a sample can be dropped. The range of possible applications is substantially widened to include asymmetric and even disordered systems as candidates. Considering, e.g., the density and sound velocity of vitreous silica and the strain coupling $\gamma \approx 2 eV$ of its intrinsic tunneling systems [24], dynamical localization may be achieved by ultrasonic driving at low temperature. At a frequency of 1 GHz, the required amplitude for localization will be reached at an acoustic intensity of about 4 mW/cm$^2$. Another phenomenon recently predicted and proposed as a testbed for theories of dissipative tunneling is the tunneling of a single atom between an STM or AFM tip and a sample [18]. The adsorbed atom forms dipoles of opposite direction on the sample and tip surfaces and thus experiences a force from an applied DC or AC tip voltage. For the Ni:Xe tunneling system proposed in [18] and characterized in more detail in [25], the localization condition for a 10 GHz driving frequency will be reached with an AC tip voltage of only about 2 mV.

This research has been supported by the National Science Foundation under grants CHE-9257094 and CHE-9528121, by the Sloan Foundation and by the Dreyfus Foundation. Computational resources have been provided by the IBM Corporation under the SUR Program at USC. J. S. enjoyed stimulating discussions with M. Grifoni and U. Weiss.

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FIG. 1. (a) Time-dependent population $p(t)$ for symmetric (dashed line) and asymmetric ($\epsilon_0 = \Delta$, solid line) tunneling systems with $\omega = 5\Delta$, and $\dot{\epsilon}/\omega = 2.38$. (b) Asymmetric system (solid lines): Non-periodic trajectories $p_n(t)$ (thin) with periodic upper and lower envelope (thick) vs. $\Delta t$. Symmetric system (dashed line): Periodic $p(t)$ of the dynamically localized system at $\dot{\epsilon}/\omega \approx 2.393$.

FIG. 2. Lower population bound $p_{\text{min}}$ vs. bias $\epsilon_0$ for various ratios $\dot{\epsilon}/\omega$ at $\omega = 5$ (unit $\Delta = 1$).

FIG. 3. Population decay for weak dissipation ($\alpha = 0.01$, zero temperature) with driving at $\omega = 5\Delta$, $\dot{\epsilon}/\omega = 2.3$, and $\omega_c = 200\Delta$. Top curve – biased system: localized, long population decay time. Middle curve – symmetric system: coherent population transfer. Lower curve – biased system, no driving: fast tunneling oscillations and incoherent decay.

FIG. 4. Slow population decay of a localized tunneling system driven at $\omega = 5\Delta$, with weak dissipation ($\alpha = 0.01$, zero temperature). Top: $\epsilon_0 = -1$, $\dot{\epsilon}/\omega = 2.3$. Center: $\epsilon_0 = 0$, $\dot{\epsilon}/\omega \approx 2.393$. Bottom: $\epsilon_0 = 1$, $\dot{\epsilon}/\omega = 2.3$. 

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