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RAPID COMMUNICATIONS

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Stabilizing coherent destruction of tunneling

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The localization of a tunneling particle by means of an oscillating external field is examined for an arbitrary doublet of tunneling states. The condition of degenerate Floquet levels, required for localization in a symmetric system, can be substantially relaxed for tunneling systems with broken symmetry. A synergistic effect of dynamic and static asymmetry is found, which extends the localization regime substantially. This generalization equally applies to tunneling systems coupled to a dissipative environment. [S1063-651X(99)50505-9]

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A tunneling particle can be localized indefinitely by an external periodic force. This surprising prediction was recently made by Grossmann *et al.* [1,2], who termed this effect coherent destruction of tunneling (CDT). 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 that 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 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,'' which is different for each driving frequency.

In this Rapid Communication, it is shown that the tunneling particle can remain trapped in a biased system, driven at a frequency and amplitude that do not match the magic numbers. This localization is a phenomenon that occurs in a parameter regime where neither the bias nor the driving force by itself can suppress tunneling. Our results strongly suggest that a generalized CDT effect can be observed in a class of systems that is much wider than previously thought. These include tunneling systems that are not intrinsically symmetric, such as the tunneling of an atom between a sample and a scanning tunnel microscope (STM) tip [17], or tunneling in disordered systems, such as structural glasses [18,19]. 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, one can either use a double-well potential model [1] or, more simply, a truncated two-state Hamiltonian [2]

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

This truncation is valid if all parameters are small compared to the lowest oscillation frequency ω_{osc} associated with the double well, for a barrier height larger than $\hbar\omega_{\mathrm{osc}}$, and for temperatures low enough to exclude the thermal excitation of higher states. σ_x and σ_z are Pauli spin matrices, $\hbar\Delta$ is the tunnel splitting, $\hbar\varepsilon_0$ is an energy bias, and $\hbar\hat{\varepsilon}\sin\omega t$ is its modulation by an external periodic force. The eigenstates $|\pm\rangle$ of σ_z form a basis of localized wave functions.

The Hamiltonian (1) is nonconservative, 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 [1–5] 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*. For large

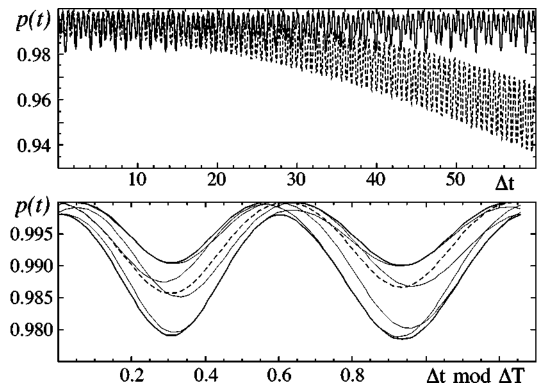

FIG. 1. (a) Time-dependent population $p(t)$ for symmetric (dashed line) and asymmetric ($\varepsilon_0=\Delta$, solid line) tunneling systems with $\omega=5\Delta$ and $\hat{\varepsilon}/\omega=2.38$. (b) *Asymmetric* system (solid lines); nonperiodic $p(t)$ (thin lines) with upper and lower envelope (thick lines). *Symmetric* system (dashed line); periodic $p(t)$ of the localized system at $\hat{\varepsilon}/\omega\approx 2.393$.

enough driving frequency, the population $p(t)$ of the initially occupied site exhibits only small oscillations during a periodicity interval, with a minimum $p_{\rm min}$ such that $|1-p_{\rm min}|\ll 1$.

In this Rapid Communication, we shall consider this inequality as the definition of a generalization of this effect, which we shall call nondegenerate coherent destruction of tunneling (NCDT) in the following. No assumptions are made about the Floquet spectrum of U_T. In this case, $p_{\rm min}$ is to be defined as the largest lower bound (infimum) of $p(t)$ for any positive t,

$$p_{\rm min}=\inf_{t\geqslant 0} p(t). \tag{2}$$

Using the group properties of discrete time translations, the dynamics at arbitrary time t can be constructed from the time-translation operator at times $\tau\leqslant T$, $U_t=U_\tau U_T^m$. Here, $U_t=U(t,0)$, with $t=mT+\tau$, $\tau\in[0,T]$, and m is an integer. The lower bound $p_{\rm min}$ is now given by

$$p_{\rm min}=\min_{0\leqslant\tau\leqslant T}\ \inf_{m\geqslant 0} p_m(\tau), \tag{3}$$

$$p_m(\tau)=\langle +|U_\tau U_T^m|+\rangle\langle +|U_T^{-m}U_\tau^\dagger|+\rangle. \tag{4}$$

For a symmetric system driven at frequencies $\omega\gg\Delta$, $p_{\rm min}$ has been shown to be almost unity if the ratio $\hat{\varepsilon}/\omega$ belongs to a set of discrete ''magic numbers'' for which U_T is diagonal and its eigenstates are degenerate [1,2]. 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 slow oscillations in $p(t)$ with large amplitude and a reduced tunneling frequency $\Delta J_0(\hat{\varepsilon}/\omega)$ will occur.

The central finding of this work is that the instability of the localization effect can be suppressed by even a very small static bias or asymmetry ε_0 of the tunneling system. This is demonstrated by the numerical data in Fig. 1. As shown in Fig. 1(a), a slight detuning of the amplitude from its magic value leads to a slow coherent transition that depopulates the initial state of a symmetric system (dashed curve). Adding a small bias, however, prevents this depopulation (solid curve). Figure 1(b) shows the corresponding set of one-period segments $p_m(\tau)$ of the curve $p(t)$ for $0\leqslant m\leqslant 3$. The $p_m(\tau)$ are bounded by lower and upper envelope functions $p_{\rm le}(\tau)$ and $p_{\rm ue}(\tau)$. These envelope functions, which are discussed in further detail below, apply to the infinite set $\{p_m(\tau)\}$ and can thus be used to establish $p_{\rm min}$. The periodic function $p(t)$ for the corresponding symmetric system with perfectly tuned amplitude $\hat{\varepsilon}/\omega\approx 2.393$ is given for comparison (dashed curve). Both cases show roughly equal $p_{\rm min}$.

It is important to note here that the minimization with respect to m can be performed exactly for any given matrix elements of U_T without extrapolating from finite to infinite m. The SU(2) matrix U_T can be represented by a generator g and an angle φ_0. This allows us to rewrite the propagation by m periods as

$$U_T^m=\exp\left(\frac{i}{2}m\varphi_0 g\right), \tag{5}$$

where g is a linear combination of the Pauli spin matrices σ_j, parameterized by a unit vector $\vec{n}$ through $g=\vec{n}\cdot\vec{\sigma}$. This illustrates the one-to-one correspondence between the conjugation term $U_T^m|+\rangle\langle +|U_T^{-m}$ in Eq. (4) and a rotation with axis $\vec{n}$ and angle $m\varphi_0$, applied to a spin vector pointing in the z direction. Because $U_T^m|+\rangle\langle +|U_T^{-m}$ can be understood to be a 2π-periodic *continuous* function of the angle $m\varphi_0$, it makes sense to define a quantity closely related to $p_m(\tau)$,

$$\tilde{p}_\varphi(\tau)=\langle +|U_\tau\exp\left(\frac{i}{2}\varphi g\right)|+\rangle\langle +|\exp\left(-\frac{i}{2}\varphi g\right)U_\tau^\dagger|+\rangle, \tag{6}$$

where the same generator g is used, but the discrete values $m\varphi_0$ of the angle are replaced by a continuous variable φ. The set of functions $\{p_m(\tau)\}$ is contained as a subset in $\{\tilde{p}_\varphi(\tau)\}$, i.e.,

$$\min_{0\leqslant\varphi\leqslant 2\pi}\tilde{p}_\varphi(\tau)\leqslant\inf_{m\geqslant 0}p_m(\tau). \tag{7}$$

For generic parameters, φ_0/π is an irrational number. The angles $m\varphi_0$ and taken modulo 2π then form a dense subset of the interval $[0,2\pi]$ and, therefore, strict equality holds in Eq. (7). But in the degenerate case of rational φ_0/π, the situation is different. The function $p(t)$ is periodic, and there are only a finite number of functions $p_m(\tau)$ that are distinct. We shall consider the latter case less relevant in the long-time limit, because any minute drift or other aberration in the driving frequency or amplitude will reduce it to the generic, nondegenerate case. Only the latter case is treated in the following.

For the two-state system, $\tilde{p}_\varphi(\tau)$ is a continuous function of φ and τ, taking the form $\tilde{p}_\varphi(\tau)=a_\tau+b_\tau\sin\varphi+c_\tau\cos\varphi$. The coefficients a_τ, b_τ, and c_τ are *algebraic functions* of the matrix elements of U_T and U_τ. When these matrix elements are given, the minimization, with respect to φ, can be performed in closed form, giving us exact, rigorous results for the lower (and upper) envelope of the set of curves $p_m(\tau)$,

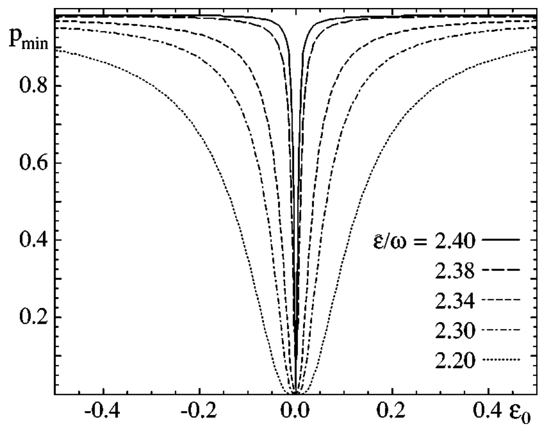

FIG. 2. Lower population bound $p_{\min}$ vs bias ε_0 for various ratios $\hat{\varepsilon}/\omega$ at $\omega=5$ (unit $\Delta=1$).

$$p_{\mathrm{le}}(\tau)=\inf_{m\geq 0} p_m(\tau)=\min_{0\leq\varphi\leq 2\pi} \tilde{p}_{\varphi}(\tau). \tag{8}$$

According to Eq. (3), $p_{\min}$ is then given by the minimum of the lower envelope, $p_{\min}=\min_{0\leq\tau\leq T} p_{\mathrm{le}}(\tau)$. The significance of Eq. (8) lies in the fact that it allows the lower population bound $p_{\min}$ for *infinite* time to be deduced from the dynamics within a *single period* of the driving force. It is through this relationship that a numerical evaluation of the Schrödinger equation yields unambiguous results for $p_{\min}$.

How large does the bias need to be in order to effect localization, and is there a maximum allowable value for this bias? The precise answer depends quite sensitively on the driving parameters. We can easily obtain the answer using the formalism outlined above. The global minimum of $p_{\mathrm{le}}(\tau)$ can be obtained by linear search because $p_{\mathrm{le}}(\tau)$ is smooth and τ is restricted to a finite interval. Figure 2 presents quantitative results about the dependence of $p_{\min}$ on ε_0 for different $\hat{\varepsilon}$ in a tunneling system driven at $\omega=5\Delta$. The width of the minimum at $\varepsilon_0=0$ vanishes as $\hat{\varepsilon}/\omega$ 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, $\varepsilon_0\approx\omega$, $p_{\min}$ drops drastically, and the dynamics is then characterized by large oscillations [8].

A basic physical understanding of this generalized localization effect can be gained by evaluating the dynamics at finite time analytically in the limit of high frequency [3,6]. For $\omega\gg\max(\varepsilon_0,\Delta)$, we find that the spin rotation for a period of the driving force has a small rotation angle $|\varphi_0|\ll 1$ and an axis $\vec{n}=N^{-1}(J_0(\hat{\varepsilon}/\omega),0,\varepsilon_0/\Delta)$. From this we conclude that localization is possible in two cases: If $\varphi_0=0$, we have the case of degenerate Floquet levels (CDT), and the tunneling system returns to its exact original state at multiples of the driving period. If, on the other hand, $0<|J_0(\hat{\varepsilon}/\omega)|\ll|\varepsilon_0/\Delta|$ (NCDT), the axis of rotation is so closely aligned with the initial spin vector that the *z* projection of the spin vector becomes virtually independent of the angle of rotation. In the latter case, the population numbers of the two tunneling sites show only extremely small oscillations, which remain negligible at all times. Although similar in origin, the two effects thus show a subtle difference. This becomes transparent when concentrating on the behavior at multiples of the driving period; in CDT, one directly observes that the effective tunneling *frequency* vanishes, while it is the *amplitude* of tunneling oscillations that becomes negligible in NCDT.

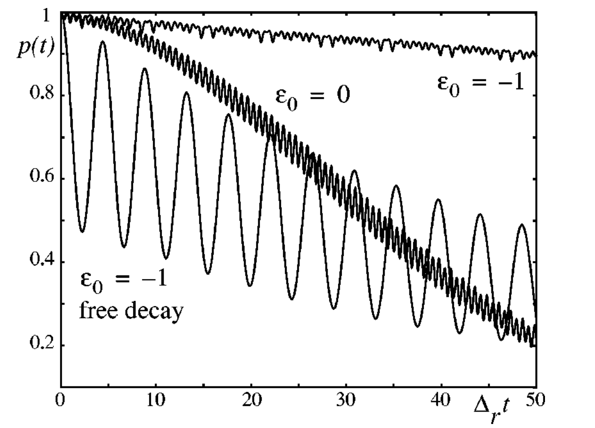

FIG. 3. Population decay for weak dissipation ($\alpha=0.01$, zero temperature) with driving at $\omega=5\Delta_r$, $\hat{\varepsilon}/\omega=2.3$, and $\omega_c=200\Delta_r$. Top curve biased system: localized, long population decay time. Middle curve, symmetric system: coherent population transfer.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

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 [20,21],

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

Here, and in the following, $\hbar=1$; q_0 is the distance between tunneling sites. The effect of the harmonic environment is fully characterized by the spectral density $J(\omega')=\pi\Sigma_\nu C_\nu^2\delta(\omega'-\omega_\nu)$. 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 [20,21]. q_0 and η appear in the dynamics only through the dimensionless dissipation constant $\alpha=\eta q_0^2/2\pi$.

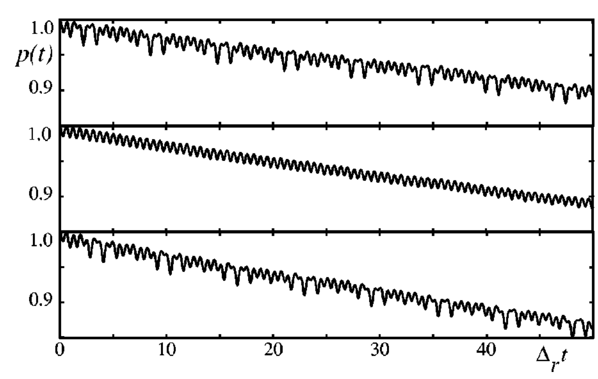

FIG. 4. Slow population decay of a localized tunneling system driven at $\omega=5\Delta_r$ with weak dissipation ($\alpha=0.01$, zero temperature). Top, $\varepsilon_0=-1$, $\hat{\varepsilon}/\omega=2.3$; center, $\varepsilon_0=0$, $\hat{\varepsilon}/\omega\approx 2.393$; bottom, $\varepsilon_0=1$, $\hat{\varepsilon}/\omega=2.3$.

In the case of large ω_c applicable to tunneling in solid-state systems, Δ and ω_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 [20,21] 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 algorithm [22] makes possible the exact and efficient computation of all dynamical quantities of interest in the spin-boson system.

The dynamics at low temperature and weak damping closely resembles that of the undamped system. Figure 3 illustrates localization in a weakly damped asymmetric tunneling system with $\hat{\varepsilon}/\omega = 2.3$ 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 $\varepsilon_0 = -1$ is introduced. The system now exhibits a gradual population decay on a much longer time scale. A comparison with the free population decay of the biased system (without driving) shows that the bias ε_0 by itself 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. Figure 4 shows the same driven system with $\varepsilon_0 = -1$ (top) and $\varepsilon_0 = 1$ (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, $\hat{\varepsilon}/\omega \approx 2.393$. Evidently, the two cases of localization discussed above lead to nearly identical behavior in the dissipative case also.

We have demonstrated that the remarkable effect of CDT can be generalized for tunneling systems having a wide range of parameters that do not obey the restrictive conditions for an exact Floquet level crossing. A synergistic effect of static asymmetry and harmonic driving permits localization in parameter regimes where neither one by itself could achieve localization. These findings improve the prospects of experimental investigation of NCDT. 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 [23]. 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], NCDT 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 atomic force microscopy tip and a sample [17]. 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 [17] 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.

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[1] F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, Phys. Rev. Lett. **67**, 516 (1991); F. Grossmann, P. Jung, T. Dittrich, and P. Hänggi, Z. Phys. B **84**, 315 (1991).
[2] F. Grossmann, and P. Hänggi, Europhys. Lett. **18**, 571 (1992).
[3] J.M. Llorente and J. Plata, Phys. Rev. A **45**, R6958 (1992); Phys. Rev. E **49**, 3547E (1994).
[4] Y. Kayanuma, Phys. Rev. A **50**, 843 (1994).
[5] L. Wang and J. Shao, Phys. Rev. A **49**, R637 (1994).
[6] H. Wang and X.-G. Zhao, J. Phys.: Condens. Matter **7**, L89 (1995); Phys. Lett. A **217**, 225 (1996).
[7] Yu. Dakhnovskii and R. Bavli, Phys. Rev. B **48**, 11 010 (1993).
[8] Yu. Dakhnovskii, R. Bavli, and H. Metiu, Phys. Rev. B **53**, 4657 (1996).
[9] T. Dittrich, B. Oelschlägel, and P. Hänggi, Europhys. Lett. **22**, 5 (1993); B Oelschlägel, T. Dittrich, and P. Hänggi, Acta Phys. Pol. B **24**, 845 (1993).
[10] F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, J. Stat. Phys. **70**, 229 (1993).
[11] Yu. Dakhnovskii, Phys. Rev. B **49**, 4649 (1994); Ann. Phys. (N.Y.) **230**, 145 (1994); J. Chem. Phys. **100**, 6492 (1994); Yu. Dakhnovskii and R.D. Coalson, *ibid.* **103**, 2908 (1995).
[12] M. Grifoni, M. Sassetti, P. Hänggi, and U. Weiss, Phys. Rev. E **52**, 3596 (1995).
[13] M. Grifoni, M. Sassetti, and U. Weiss, Phys. Rev. E **53**, R2033 (1996).
[14] M. Grifoni and P. Hänggi, Phys. Rep. **304**, 229 (1998).
[15] D.E. Makarov and N. Makri, Phys. Rev. E **52**, 5863 (1995); N. Makri, J. Chem. Phys. **106**, 2286 (1997).
[16] P. Neu and J. Rau, Phys. Rev. E **55**, 2195 (1997).
[17] A.A. Louis and J.P. Sethna, Phys. Rev. Lett. **74**, 1363 (1995).
[18] P. Anderson, B. Halperin, and C. Varma, Philos. Mag. **25**, 1 (1972).
[19] W. Phillips, J. Low Temp. Phys. **7**, 351 (1972).
[20] A.J. Leggett, S. Chakravarty, A.T. Dorsey, M.P.A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987); *ibid.* **67**, 725 (1995).
[21] U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 1993), and references therein.
[22] J.T. Stockburger and C.H. Mak, Phys. Rev. Lett. **80**, 2657 (1998).
[23] This generalization depends on a successful two-state description of tunneling (cf. Refs. [18,19]).
[24] J.E. Graebner, L.C.A. Golding, and A.B. Kane, Phys. Rev. B **27**, 3697 (1983).
[25] R.E. Walkup, D.M. Newns, and Ph. Avouris, Phys. Rev. B **48**, 1858 (1993).