Landau-Zener-Stueckelberg Physics with a Singular Continuum of States

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(Received 13 September 2016; published 6 January 2017)

This Letter addresses the dynamical quantum problem of a driven discrete energy level coupled to a semi-infinite continuum whose density of states has a square-root-type singularity, such as states of a free particle in one dimension or quasiparticle states in a BCS superconductor. The system dynamics is strongly affected by the quantum-mechanical repulsion between the discrete level and the singularity, which gives rise to a bound state, suppresses the decay into the continuum, and can produce Stueckelberg oscillations. This quantum coherence effect may limit the performance of mesoscopic superconducting devices, such as the quantum electron turnstile.

DOI: 10.1103/PhysRevLett.118.016805

The Landau-Zener (LZ) transition between two coupled quantum states whose energies cross in time is a paradigmatic situation in quantum mechanics. Because of its generality and simplicity, the LZ model, originally proposed to describe atomic collisions [1–3] and spin dynamics in a magnetic field [4], was later applied to many different phenomena, such as electron transfer in donor-acceptor complexes [5], spin dynamics in magnetic molecular clusters [6], molecular production in cold atomic gases [7], electron pumping [8] and capture [9] in quantum dots, dissipation in driven mesoscopic rings [10], or in superconductor tunnel junctions [11,12]. In the course of intense research in various fields, several generalizations of the two-level LZ model to multiple levels have been found [13–21] including finite-time exact solutions [22,23], and even many-body versions of the LZ model have been considered [7,24–26]. However, these generalizations still deal with discrete energy levels. A notable exception is Ref. [13], whose authors analyzed a single discrete level driven linearly through an arbitrary spectrum, which could also be continuous.

In the present Letter, I present another extension of the Landau-Zener problem involving a discrete level coupled to a continuum of states, which has an approximate analytical solution in the long-time limit. The continuum states are assumed to have positive energies, $E > 0$, with the density of states (DOS) $\nu(E)$ having a singularity $\nu(E) \propto 1/\sqrt{E}$ at $E \to 0^+$. This singularity is the essential ingredient of the problem. Physically, such a continuum can be represented by a one-dimensional wire with the parabolic dispersion, or by quasiparticle states in a BCS superconductor above the superconducting gap. The discrete level (located on an impurity or a small quantum dot) initially has large negative energy and contains one particle. Then, its energy E_d is moved inside the continuum (e.g., by applying a gate voltage), where it stays for some time, and then is driven back to large negative energies, as shown in Fig. 1 by the dashed line. The quantity of interest is the probability p_∞ for the particle to stay on the discrete level without being ejected into the continuum. A related problem of a vanishing bound state in atom-ion collisions was considered in Ref. [27].

The practical motivation for the present study comes from the quantum electron turnstile, a nanoelectronic device transferring electrons one by one, with a potential metrological application as a current standard (see reviews [28,29]). The electron transfer occurs via a small metallic nanoparticle sandwiched between two superconducting electrodes [30]. For a small enough particle, the electron confinement is very strong, so there is effectively a single electronic level whose double occupancy is prohibited by the Coulomb repulsion, and whose energy is controlled by a nearby gate electrode [31,32]. The key step of the operation is the electron ejection from the nanoparticle level, driven by the gate voltage, into the empty quasiparticle states on one of the superconducting electrodes. If the

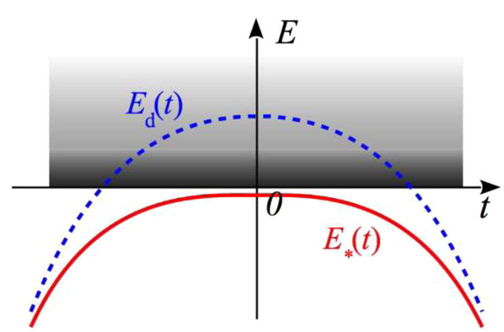

FIG. 1. A sketch of the time dependence of various energies. The gray area at $E > 0$ represents the continuum with the singularity in the DOS at $E \to 0$. The dashed blue line shows the bare discrete level $E_d(t)$, driven inside the continuum for a finite time. The solid red line shows the adiabatic ground state $E_*(t)$.

superconducting gap is large enough, one can consider the single-particle problem. The level trajectory then corresponds to that shown in Fig. 1, with the energy counted from the BCS singularity. The survival probability p_∞ contributes to the turnstile operation error.

The standard description of the decay into a continuum is by the perturbative Fermi golden rule, which gives the decay rate $\Gamma(E_d)$ for a fixed level energy E_d. Application of the golden rule at each instant of time gives

$$p_\infty = \exp\left(-\int_{E_d(t)>0} \Gamma(E_d(t))dt\right), \qquad (1)$$

where the integration is over the time interval during which the level stays inside the continuum. Obviously, Eq. (1) is not valid for a too fast drive leading to a large energy uncertainty. Much less obvious is the breakdown of the quasistationary Eq. (1) at slow drive. It is the main focus of the present Letter.

The key fact is that for a fixed E_d, the exact eigenstates of the coupled system form a continuum at $E > 0$, and in addition, there is a discrete bound state at an energy $E = E_* < 0$ [33–35], similar to the Yu-Shiba-Rusinov states bound to a magnetic impurity [36–39]. For large negative E_d, the bound state approximately coincides with the bare discrete level, $E_* \approx E_d$. For $E_d > 0$, no matter how large, the bound state with $E_* < 0$ still exists, although for $E_d \to +\infty$ its energy approaches the continuum and its overlap with the bare discrete state vanishes. The existence of the bound state is a consequence of the DOS singularity at $E \to 0^+$ and can be viewed as due to the quantum-mechanical repulsion between the bare level and the singularity. As the bound state is the adiabatic ground state of the coupled system, for slow drive the particle will always stay in it, implying $p_\infty \to 1$.

To describe the crossover between the regime of Eq. (1) and the adiabatic regime with $p_\infty \to 1$, one has to analyze the dynamical problem. Below, its analytical solution is presented for a special case of the parabolic time dependence $E_d(t)$, obtained by adapting the method of Demkov and Osherov [13]. Remarkably, the survival probability has the two-path structure $p_\infty = |A_d + A_*|^2$, where A_d corresponds to the resonance in the continuum (the dashed line in Fig. 1) with $|A_d|^2$ decaying according to Eq. (1), while the nondecaying A_* is the contribution of the adiabatic ground state (the solid line in Fig. 1). The cross term in p_∞ describes Stueckelberg-like interference between the two paths, leading to an oscillatory dependence of p_∞ on the drive parameters. Indeed, the bound state may be viewed as a result of avoided crossing between the discrete level and the singularity; the double passage of this crossing is similar to the Stueckelberg interferometer.

The model.—In a BCS superconductor, the quasiparticle DOS is given by $\nu(\epsilon) = \nu_0\theta(|\epsilon| - \Delta)|\epsilon|/\sqrt{\epsilon^2 - \Delta^2}$, where ν_0 is the normal-state DOS, the energy ϵ is counted from the Fermi level, 2Δ is the superconducting gap, and $\theta(\epsilon)$ is the step function. In the vicinity of the BCS singularity at $\epsilon \to \Delta$, the quasiparticle energy, counted from Δ (it is convenient to shift the energy reference as $E = \epsilon - \Delta$), can be approximated as $E_k = \sqrt{\xi_k^2 + \Delta^2} - \Delta \approx \xi_k^2/(2\Delta)$, and the Bogolyubov quasiparticle factors $u_k \approx v_k \approx 1/\sqrt{2}$. Here the index k labels the quasiparticle states, and ξ_k are the normal-state quasiparticle energies, so that the state summation $\sum_k$ is represented as $\nu_0 \int d\xi_k$. The particle wave function has a component ψ_d on the bare discrete level, and components ϕ_k on the continuum states. They satisfy the two components of the Schrödinger equation (we set $\hbar = 1$):

$$i\frac{d\psi_d}{dt} = E_d(t)\psi_d + \sqrt{\frac{\gamma_0}{2\pi\nu_0}}\phi_k, \qquad (2)$$

$$i\frac{d\phi_k}{dt} = \frac{\xi_k^2}{2\Delta}\phi_k + \sqrt{\frac{\gamma_0}{2\pi\nu_0}}\psi_d, \qquad (3)$$

where the coupling strength is parametrized by $2\gamma_0$, the energy-independent decay rate in the normal state. These equations can be equivalently rewritten in the coordinate representation, $\phi_k = \int \phi(x)e^{ikx}dx$, $\xi_k^2 \to -v_F^2\partial_x^2$, where v_F is the Fermi velocity; then they become identical to the Schrödinger equation for a simple one-dimensional wire coupled to a discrete site at $x = 0$.

The exact eigenstate energies for fixed E_d are found by substituting $i(d/dt) \to E$ and eliminating ϕ_k. This gives the equation $G_d^{-1}(E) = 0$, where the bare discrete level Green's function and the self-energy are defined as

$$G_d(E) = \frac{1}{E - E_d - \Sigma(E)}, \qquad \Sigma(E) = -\sqrt{\frac{\gamma_0^2\Delta}{-2E}}. \qquad (4)$$

$\Sigma(E > 0)$ is imaginary, describing the particle escape from the discrete level into the continuum with the rate $\Gamma(E) = -2\mathrm{Im}\Sigma(E + i0^+)$. $\Sigma(E < 0)$ is real and negative, describing the quantum-mechanical level repulsion. The divergence of $\Sigma(E \to 0^-)$ results in the existence of a real solution of $G_d^{-1}(E) = 0$ with $E = E_* < 0$ for any E_d. Thus, the spectrum consists of a discrete bound state at $E = E_*$, represented by the isolated pole of $G_d(E)$, and of the continuum at $E > 0$, corresponding to the branch cut of $\sqrt{-E}$. The weight of the bare discrete level in the exact bound state is given by the residue Z of $G_d(E)$ in the pole $E = E_*$. For positive $E_d \gg (\gamma_0^2\Delta)^{1/3}$, the bound state is shallow, $E_* \approx -\gamma_0^2\Delta/(2E_d^2)$, and the weight is small, $Z \approx \gamma_0^2\Delta/E_d^3$.

Knowledge of the eigenstates at fixed E_d enables one to treat a special case when the level energy abruptly rises from $-\infty$ to a finite value E_d (a quantum quench), stays constant for a long time, and then drops back to $-\infty$. The probability amplitude on the ground state after the first quench is given by the projection of the discrete level on the ground state, $\sqrt{Z}$. After a sufficient time the continuum component is dephased, so on the second quench the bound state is projected back on the discrete state, which gives another factor $\sqrt{Z}$. The resulting survival probability (amplitude squared) is then $p_\infty = Z^2$.

Returning to the dynamical problem, we eliminate $\phi_k(t)$ from Eqs. (2), (3), and obtain an equation for $\psi_d(t)$,

$$i\frac{d\psi_d(t)}{dt} = E_d(t)\psi_d(t) + \int_{-\infty}^{t} \tilde{\Sigma}(t-t')\psi_d(t')dt', \quad (5)$$

where $\tilde{\Sigma}(t) = e^{5i\pi/4}\theta(t)\sqrt{\gamma_0^2\Delta/(2\pi t)}$ is the Fourier transform of $\Sigma(E + i0^+)$. Equation (5) should be solved with the initial condition $|\psi_d(t\to-\infty)| = 1$, and the quantity of interest is $p_\infty = |\psi_d(t\to+\infty)|^2$.

Markovian regime.—Let us pass to the interaction representation by writing $\psi_d(t) = \Psi_d(t)e^{-i\Phi(t)}$, where $\Phi(t) \equiv \int_0^t E_d(t')dt'$. Equation (5) becomes

$$i\frac{d\Psi_d(t)}{dt} = \int_{-\infty}^{t} \tilde{\Sigma}(t-t')e^{i\Phi(t)-i\Phi(t')}\Psi_d(t')dt'. \quad (6)$$

If $e^{i\Phi(t)-i\Phi(t')}$ is quickly oscillating for t' far from t, the integral converges at short $t - t'$. If the time dependence of $\Psi_d(t')$ is slow enough on the convergence time scale, one can approximate $\Psi_d(t') \approx \Psi_d(t)$ and take it out of the integral (Markovian approximation). The resulting differential equation is straightforwardly integrated to give

$$p_\infty = \exp\left(-2\int_0^\infty \frac{dE}{2\pi}\sqrt{\frac{\gamma_0^2\Delta}{2E}}|F(E)|^2\right), \quad (7)$$

where $F(E) \equiv \int e^{iEt-i\Phi(t)}dt$. Equation (1) can be obtained from Eq. (7) by calculating $F(E)$ in the stationary phase approximation, or, equivalently, by approximating $\Phi(t) - \Phi(t') \approx E_d(t)(t - t')$ in Eq. (6), whose right-hand side then becomes just $\Sigma(E_d(t))\Psi_d(t)$.

The Markovian character of the integral (6) is lost most easily at times $t \approx t_0$ when $E_d(t_0) = 0$. Approximating $\Phi(t) \approx \Phi(t_0) + \dot{E}_d(t_0)(t-t_0)^2/2 + \ddot{E}_d(t_0)(t-t_0)^3/3$, where $\dot{E}_d \equiv dE_d/dt$, $\ddot{E}_d \equiv d^2E_d/dt^2$, we obtain the condition for the validity of the Markovian approximation as $\max\{|\dot{E}_d|^{3/2}, |\ddot{E}_d|\} \gg \gamma_0^2\Delta$. If $E_d(t) < 0$ always, the validity is determined by the values $E_d(t_{\max})$, $\ddot{E}_d(t_{\max})$ at the maximum: $\max\{|E_d^3|, |\ddot{E}_d|\} \gg \gamma_0^2\Delta$.

Adiabatic regime.—The system is expected to be in the adiabatic regime as long as $|dE_*/dt| \ll E_*^2$ (as in the standard LZ theory). If this holds at all times, the probability $1 - p_\infty$ for the particle to leave the ground state is expected to be exponentially small. In this regime, solving Eq. (5), either analytically and numerically, is not an easy task. Indeed, Eq. (5) is deduced from the Schrödinger equation in the diabatic basis, which is not a natural one to describe the adiabatic regime [40]. Still, by adapting the method of Ref. [13], an analytical solution can be found for one specific case of the parabolic time dependence $E_d(t) = h - wt^2$, parametrized by the top energy h and $w > 0$ (since $\hbar = 1$ was assumed, w has the dimensionality of energy cubed).

Namely, one goes to the Fourier space,

$$\psi_d(t) = \int \frac{dE}{2\pi} e^{-iEt}\tilde{\psi}(E), \quad (8)$$

where the integration is performed over the real axis. Since $t^2 \to -d^2/dE^2$, Eq. (5) is transformed into

$$-w\frac{d^2\tilde{\psi}}{dE^2} + \left[E + \sqrt{\gamma_0^2\Delta/(-2E)}\right]\tilde{\psi} = h\tilde{\psi}, \quad (9)$$

having the form of the stationary one-dimensional Schrödinger equation with a complex potential (at $E > 0$, the square root is positive imaginary after analytical continuation in the upper complex half-plane). The solution must decay exponentially at $E \to +\infty$. At $E \to -\infty$, it has the WKB form with some coefficients C_+, C_-:

$$\tilde{\psi}(E\to-\infty) = \sum_{\pm} C_\pm \frac{e^{\pm iS(E)}}{\sqrt{S'(E)}}, \qquad S' \equiv \frac{dS}{dE}, \quad (10)$$

$$S(E) = \int^E \frac{d\varepsilon}{\sqrt{w}}\sqrt{h - \varepsilon - \sqrt{\gamma_0^2\Delta/(-2\varepsilon)}}. \quad (11)$$

At $t \to \pm\infty$, the integral in Eq. (8) can be calculated in the stationary phase approximation. For each t, only one of the two terms in Eq. (10) produces a stationary point, determined by $\pm t = S'(E) > 0$. At $|t| \to \infty$, the solution $E_t = h - wt^2 \to -\infty$, so one can indeed use the asymptotic WKB expression (10). As a result,

$$\psi_d(t\to\pm\infty) = e^{\mp i\pi/4}\sqrt{\frac{w}{\pi}}C_\pm e^{-iE_t t \pm iS(E_t)}, \quad (12)$$

which gives $p_\infty = |C_+/C_-|^2$. Thus, the survival probability p_∞ of the dynamical problem (5) corresponds to the inverse reflection coefficient in the scattering problem for the Schrödinger equation (9). The positive imaginary part of the potential ensures $p_\infty < 1$.

The adiabatic effect is nontrivial when the bound state is shallow, $h \gg (\gamma_0^2\Delta)^{1/3}$. We also assume $h^3 \gg w$; otherwise, the time spent by $E_d(t)$ in the continuum is too short (the energy uncertainty exceeds h), and $p_\infty \approx 1$ can be found from Eq. (7) with $F(E) = 2\pi w^{-1/3}\mathrm{Ai}[w^{-1/3}(E - h)]$, where $\mathrm{Ai}(x)$ is the Airy function. When $h^3 \gg w$, $\gamma_0^2\Delta$ (below the red solid line in Fig. 2), the wave function $\tilde{\psi}(E)$ can be found in the WKB approximation everywhere except (i) the vicinity of the classical turning point $E = h$, where it can be treated in the standard way, and (ii) near the singularity at $E \to 0$ (see Supplemental Material [41] for details). Then, one can identify two limiting cases for matching the WKB solution at $E \to 0$,

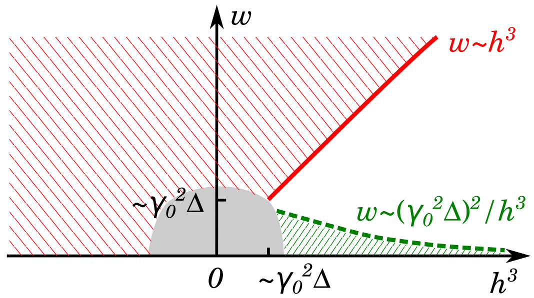

FIG. 2. Different regimes for the problem (5) with $E_d(t) = h - wt^2$. The adibatic regime with $1 - p_\infty \ll 1$ (hatched area below the dashed line) occurs if the condition $|dE_*/dt| \ll E_*^2$ holds at all times. In the fast-drive regime (hatched area to the left of the solid line), the time spent in the continuum is too short, so that h is within the energy uncertainty and $1 - p_\infty \ll 1$. In the golden rule regime (white area between the dashed and the solid line) $p_\infty \ll 1$. The gray area corresponds to $h^3 \sim w \sim \gamma_0^2\Delta$ with $p_\infty \sim 1$.

governed by the parameter $\sqrt{wh^3}/(\gamma_0^2\Delta)$. They are separated by the dashed line in Fig. 2.

(i) In the adiabatic regime, $\sqrt{wh^3} \gg \gamma_0^2\Delta$, the particle stays in the ground state up to an exponentially small ejection probability,

$$p_\infty = 1 - \exp\left(-\frac{\pi}{4}\frac{\gamma_0^2\Delta}{\sqrt{wh^3}}\right). \quad (13)$$

(ii) In the opposite limit, C_+/C_- is calculated to the first order in $\sqrt{wh^3}/(\gamma_0^2\Delta) \ll 1$, which gives

$$p_\infty = \left| e^{-\pi\sqrt{\gamma_0^2\Delta/(2w)} - (4/3)i\sqrt{h^3/w}} + e^{i\pi/4}\sqrt{\frac{\pi}{4}\frac{\gamma_0^2\Delta}{\sqrt{wh^3}}} \right|^2. \quad (14)$$

The first term [of zero order in $\sqrt{wh^3}/(\gamma_0^2\Delta)$] gives the golden rule expression (1); indeed, the exponent is nothing but $(1/2)\int\Gamma(E_d(t))dt - i\int E_d(t)dt$ for $E_d(t) = h - wt^2$. The second term is the first-order correction which must be small compared to unity, but can still be larger than the zero-order term. Remarkably, in the latter case it matches the adiabatic expression (13) obtained in the opposite limit.

Discussion.—Equations (7), (13), and (14) represent the main result of the present work. They agree with the numerical solution of Eq. (5) (see the Supplemental Material [41]). Although Eqs. (13) and (14) are obtained for a specific dependence $E_d(t) = h - wt^2$, their relevance is quite general, since any smooth $E_d(t)$ can be approximated by a parabola near the maximum. The three expressions have overlapping domains of validity: Eq. (7) with $F(E) = 2\pi w^{-1/3}\mathrm{Ai}[w^{-1/3}(E-h)]$ matches the first term in Eq. (14), while Eq. (13) matches the second. The only region not covered by Eqs. (7), (13), and (14) is $h^3 \sim w \sim \gamma_0^2\Delta$, shown in Fig. 2 by the gray area.

Equation (14) has a two-path form, corresponding to the two trajectories shown in Fig. 1. Because of the h- and w-dependent phase of the first term, p_∞ may exhibit Stueckelberg interference oscillations as a function of h or w. From the analogy with the standard two-level problem, it is tempting to assume that the crossing of the singularity at $t_0 = -\sqrt{h/w}$ can be viewed as a beam splitter, when the particle "decides" which path to follow. However, if this were the case, the system behavior would be determined by $E_d(t)$ linearized around t_0, i.e., by $\dot{E}_d(t_0) = 2\sqrt{wh}$, while in Eq. (14) the parameter governing the amplitude of the adiabatic path is $\sqrt{wh^3}/(\gamma_0^2\Delta)$. This latter parameter is nothing but the maximal value of $E_*^{-2}|dE_*/dt|$, which should be small to keep the adiabaticity at all times. This maximal value is reached at $t \approx t_0/\sqrt{3}$, quite far from the crossing.

In any realistic superconducting device, the BCS singularity in the DOS, which is the key ingredient of the problem, is necessarily smeared on some energy scale. If the smearing exceeds $|E_*|$, the bound state enters the continuum and decays, so the described effect is no longer relevant. The smearing is often quantified by the Dynes parameter [42,43], which gives the ratio of the smearing scale to the gap Δ. For aluminum-based superconducting nanostructures, the Dynes parameter is typically 10^{-4}–10^{-5}, mostly due to microwave noise from the environment [44], and can be made as low as 10^{-7} if special efforts are made to ensure efficient microwave shielding and quasiparticle relaxation [45]. Taking the values $\gamma_0 = 1\ \mu$eV, $\Delta = 200\ \mu$eV [31], we obtain the main energy scale responsible for the formation of the bound state $(\gamma_0^2\Delta/2)^{1/3} \approx 5\ \mu$eV, which exceeds the Dynes smearing by several orders of magnitude. For a sinusoidal drive with the amplitude 100 μeV and frequency 50 MHz [32], we obtain $w \approx 2\ \mu\mathrm{eV}^3$. Then the level should be pushed by $h \sim [(\gamma_0^2\Delta/2)^2/w]^{1/3} \sim$ a few μeV beyond the BCS singularity to overcome the adiabatic blocking, and the period of the Stueckelberg oscillations is $h \sim w^{1/3} \sim 1\ \mu$eV, both corresponding to quite measurable energy scales. To give a noticeable amplitude of the oscillations, w should not be too small compared to $\pi^2\gamma_0^2\Delta/2$, so it is better to use a device with sub-μeV γ_0.

The experimental resolution is more likely to be limited by the high-frequency noise component of the driven gate voltage, which should favor electron ejection from the bound state into the continuum. Thus, in experiment, special care should be taken in order to reduce this extrinsic noise. Theoretically, the effect of noise has been studied for the standard two-level Landau-Zener problem [46–51]; inclusion of noise in the present theory along the same lines is a subject for future work.

To conclude, I presented an extension of the Landau-Zener problem to a continuous energy spectrum. The key role is played by the singularity in the continuum DOS, which is crossed by the driven discrete level. The Landau-Zener physics is not washed out by the continuum because of the quantum-mechanical level repulsion between the discrete level and the DOS singularity, and even Stueckelberg oscillations are present. The fundamental physics, described here, is shown to be relevant for a specific mesoscopic device, the hybrid quantum electron turnstile, where the BCS singularity in the quasiparticle DOS of superconducting electrodes may prevent electron ejection from the discrete quantum dot level into the electrode, thereby providing a fundamental limit on the device operation.

The author is grateful to D. Van Zanten, C. Winkelmann, and H. Courtois for the stimulating discussions that initiated this work, as well as to Yu. Galperin, M. Houzet, I. Khaymovich, M. Kiselev, L. Levitov, J. Pekola, V. Pokrovsky, A. Shushin, X. Waintal, R. Whitney, E. Yuzbashyan, and many others for helpful discussions on various stages of the work.

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