Evolution of superpositions of quantum states through a level crossing

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The Landau-Zener-Stückelberg-Majorana (LZSM) model is widely used for estimating transition probabilities in the presence of crossing energy levels in quantum physics. This model, however, makes the unphysical assumption of an infinitely long constant interaction, which introduces a divergent phase in the propagator. This divergence remains hidden when estimating output probabilities for a *single* input state insofar as the divergent phase cancels out. In this paper we show that, because of this divergent phase, the LZSM model is inadequate to describe the evolution of pure or mixed *superposition* states across a level crossing. The LZSM model can be used only if the system is initially in a single state or in a completely mixed superposition state. To this end, we show that the more realistic Demkov-Kunike model, which assumes a hyperbolic-tangent level crossing and a hyperbolic-secant interaction envelope, is free of divergences and is a much more adequate tool for describing the evolution through a level crossing for an arbitrary input state. For multiple crossing energies which are reducible to one or more effective two-state systems (e.g., by the Majorana and Morris-Shore decompositions), similar conclusions apply: the LZSM model does not produce definite values of the populations and the coherences, and one should use the Demkov-Kunike model instead.

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I. INTRODUCTION

Whenever the energies of two discrete quantum states cross when plotted against some parameter (e.g., time), the transition probability is traditionally estimated by the Landau-Zener-Stückelberg-Majorana (LZSM) formula [1]. Despite its very simple time dependence—linearly changing energies and a constant interaction of infinite duration—when applied to real physical systems with more elaborate time dependencies the LZSM model often provides unexpectedly accurate results. This feature, and the extreme simplicity of the LZSM transition probability, explain the vast popularity of the LZSM model, which has become a standard tool in time-dependent quantum dynamics. Nevertheless, the unphysical nature of the LZSM model—the assumption for nonvanishing interaction at infinite times—leads to a mathematical deficiency: the LZSM propagator contains a divergent phase factor. When the two-state system is initially in a single state, this divergence is often overlooked because it does not affect the occupation probabilities.

In this paper we address a rather basic and simple problem in time-dependent quantum dynamics: how a two-state system in an arbitrary initial state propagates through a level crossing. This problem has rarely been an issue until recently, insofar as the traditional objective has been the complete or partial transfer of population between two (or more) quantum states, either by Rabi (or generalized Rabi) oscillations or adiabatic passage techniques [2]. With the rapid development of the field of quantum information, which utilizes a string of unitary operations (gates) wherein phase coherence is essential, coherent superposition states have become a common object for quantum state engineering and manipulation. Here we demonstrate that, due to its intrinsic phase divergence, the LZSM model does not allow us to determine the output state after the crossing in the general case of a superposition input state, pure or partly mixed, with nonzero initial coherences. To this end, we study in detail the most general conditions that should be fulfilled in order to have defined output density matrix elements for the LZSM model.

We show that, for a system in an arbitrary initial state with nonzero initial coherences and subjected to a level-crossing interaction, the exactly soluble Demkov-Kunike (DK) model [3] is a powerful and flexible alternative to the LZSM model because it provides definite values of the output populations and coherences. Moreover, it uses more realistic and flexible physical assumptions about the amplitude and the frequency of the external field.

This paper is organized as follows. In Sec. II we introduce the basic equations, describing the dynamics of a two-state quantum system in a general mixed state. Section III A discusses the problems and limitations of using the LZSM model. In Sec. III B we introduce the DK model, and we show that it is indeed appropriate to describe the evolution of superposition states through a level crossing. In Sec. III C we describe examples of physical systems where such problems may arise. Section IV extends our studies to systems with multiple states. The conclusions are summarized in Sec. V.

II. BACKGROUND

A. Pure states

A pure state of a coherently driven two-state quantum system is described in the interaction representation by the state vector

$$|\Psi(t)\rangle = \sum_{n=1}^{2} c_n(t) \exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right]|n\rangle, \qquad (1)$$

where $c_n(t)$ is the complex-valued probability amplitude of state $|n\rangle$. Here $E_n(t)$ are the eigenenergies of the unperturbed Hamiltonian $\mathbf{H}_0(t)$, which can generally be time dependent,

$$\mathbf{H}_0(t)|n\rangle = E_n(t)|n\rangle. \qquad (2)$$

The time dependence in $\mathbf{H}_0(t)$, and consequently in $E_n(t)$, may occur due to the accidental presence, or the deliberate application, of time-dependent energy-shifting external fields, which cause Zeeman or Stark shifts: $E_n(t) = E_n^0 + E_n^Z(t) + E_n^S(t)$. These shifts will modify the Bohr transition frequency $\omega_0(t) = [E_2(t) - E_1(t)]/\hbar$.

The full Hamiltonian includes the (generally time-dependent) interaction $\mathbf{V}(t)$: $\mathbf{H}(t) = \mathbf{H}_0(t) + \mathbf{V}(t)$. The amplitudes $c_1(t)$ and $c_2(t)$ are solutions of the two-state Schrödinger equation,

$$i\hbar \frac{d}{dt}\mathbf{c}(t) = \mathbf{H}(t)\mathbf{c}(t), \tag{3}$$

where $\mathbf{H}(t)$ is the Hamiltonian of the system and $\mathbf{c}(t) = [c_1(t), c_2(t)]^T$. In the interaction representation (1), the Schrödinger equation reduces to two coupled equations,

$$i\frac{d}{dt}c_1(t) = \frac{1}{2}\Omega(t)e^{-i\mathcal{D}(t)}c_2(t), \tag{4a}$$

$$i\frac{d}{dt}c_2(t) = \frac{1}{2}\Omega(t)e^{i\mathcal{D}(t)}c_1(t). \tag{4b}$$

Here $\mathcal{D}(t) = \int_0^t \Delta(t')dt'$ is an integral over the frequency detuning $\Delta(t) = \omega_0(t) - \omega(t)$, which is the difference between the Bohr transition frequency $\omega_0(t)$ and the laser carrier frequency $\omega(t)$. For laser-driven atomic or molecular transitions, $\Omega(t) = -\mathbf{d}\cdot\mathbf{E}(t)/\hbar$ is the Rabi frequency, where $\mathbf{d}$ is the transition dipole moment and $\mathbf{E}(t)$ is the envelope of the laser electric field. In nuclear magnetic resonance, the Rabi frequency is proportional to the magnetic moment of the spin $\boldsymbol{\mu}$ and the external magnetic field $\mathbf{B}(t)$, $\Omega(t) = -\boldsymbol{\mu}\cdot\mathbf{B}(t)/\hbar$.

We assume that, at a certain time t_i, the two-state system is in the coherent superposition

$$|\Psi_\mathrm{i}\rangle \equiv |\Psi(t_\mathrm{i})\rangle = c_1|1\rangle + c_2|2\rangle, \tag{5}$$

We note that this superposition can be stable in time (no relative phase induced by free evolution) only if the two states $|1\rangle$ and $|2\rangle$ are degenerate, for example, if the system is formed of two ground atomic states in a Raman linkage. Otherwise, free evolution must be accounted for in any subsequent change of the superposition.

A Hermitian Hamiltonian induces unitary evolution between an initial state $|\Psi_\mathrm{i}\rangle$ and a final state $|\Psi_\mathrm{f}\rangle$:

$$|\Psi_\mathrm{f}\rangle = \mathbf{U}(t_\mathrm{f},t_\mathrm{i})|\Psi_\mathrm{i}\rangle, \tag{6}$$

where $\mathbf{U}(t_\mathrm{f},t_\mathrm{i})$ is the propagator of the system. Because of its SU(2) symmetry, the propagator can be parametrized by using the Cayley-Klein parameters a and b,

$$\mathbf{U}(\infty,-\infty) = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix}. \tag{7}$$

Alternatively, the propagator can be parametrized in terms of the Stückelberg variables,

$$\mathbf{U}(\infty,-\infty) = \begin{bmatrix} e^{i\theta}\sqrt{1-p} & e^{i\phi}\sqrt{p} \\ -e^{-i\phi}\sqrt{p} & e^{-i\theta}\sqrt{1-p} \end{bmatrix}, \tag{8}$$

where $p = |b|^2$ is the transition probability, while θ and ϕ are the Stückelberg phases. Obviously, $a = e^{i\theta}\sqrt{1-p}$ and $b = e^{i\phi}\sqrt{p}$.

For time-symmetric coupling, $\Omega(-t) = \Omega(t)$, and for antisymmetric detuning, $\Delta(-t) = -\Delta(t)$, as it is the case in the LZSM model, one can show by using the symmetry of the Schrödinger equation that $\mathrm{Im}U_{11} = \mathrm{Im}U_{22} = 0$ [4]. We will use the Stückelberg parametrization for the LZSM model, while the Cayley-Klein parametrization will be used for the DK model.

B. Mixed states

A mixed state of the system is described by a density matrix $\boldsymbol{\rho}$. The evolution of a mixed state $\boldsymbol{\rho}^\mathrm{i}$ under a Hermitian Hamiltonian, which generates a unitary propagator $\mathbf{U}$, is unitary,

$$\boldsymbol{\rho}^\mathrm{f} = \mathbf{U}\boldsymbol{\rho}^\mathrm{i}\mathbf{U}^\dagger, \tag{9}$$

where $\boldsymbol{\rho}^\mathrm{f}$ is the final mixed state. Using Eqs. (7) and (9) we obtain the elements of the final density matrix,

$$\rho_{11}^\mathrm{f} = |a|^2\rho_{11}^\mathrm{i} + |b|^2\rho_{22}^\mathrm{i} + 2\mathrm{Re}\big[ab^*\rho_{12}^\mathrm{i}\big], \tag{10a}$$

$$\rho_{22}^\mathrm{f} = 1 - \rho_{11}^\mathrm{f}, \tag{10b}$$

$$\rho_{12}^\mathrm{f} = ab\big(\rho_{22}^\mathrm{i} - \rho_{11}^\mathrm{i}\big) + a^2\rho_{12}^\mathrm{i} - b^2\rho_{21}^\mathrm{i}, \tag{10c}$$

$$\rho_{21}^\mathrm{f} = \big(\rho_{12}^\mathrm{f}\big)^*. \tag{10d}$$

In Stückelberg variables, Eq. (8), we have

$$\rho_{11}^\mathrm{f} = (1-p)\rho_{11}^\mathrm{i} + p\rho_{22}^\mathrm{i} + 2\sqrt{p(1-p)}\mathrm{Re}\big[\rho_{21}^\mathrm{i}e^{i\phi}\big], \tag{11a}$$

$$\rho_{22}^\mathrm{f} = 1 - \rho_{11}^\mathrm{f}, \tag{11b}$$

$$\rho_{12}^\mathrm{f} = \sqrt{p(1-p)}\big(\rho_{22}^\mathrm{i} - \rho_{11}^\mathrm{i}\big)e^{i\phi} + (1-p)\rho_{12}^\mathrm{i} - e^{2i\phi}p\rho_{21}^\mathrm{i}, \tag{11c}$$

$$\rho_{21}^\mathrm{f} = \big(\rho_{12}^\mathrm{f}\big)^*, \tag{11d}$$

where $\theta = 0$ is assumed. We shall show now that for the LZSM model [1], these density matrix elements are not always defined.

III. EVOLUTION OF SUPERPOSITION STATES THROUGH LEVEL CROSSING

A. LZSM model

The LZSM model assumes a constant coupling and a linearly changing detuning,

$$\Omega(t) = \Omega_0, \quad \Delta(t) = Ct, \tag{12}$$

where Ω_0 and C are assumed to be real positive constants and the coupling Ω lasts from $t \to -\infty$ to $t \to \infty$. In terms of the dimensionless parameters

$$\Lambda = \frac{\Omega_0^2}{C}, \quad \tau_{\mathrm{i,f}} = C^{\frac{1}{2}}t_{\mathrm{i,f}}, \tag{13}$$

the parameters in the propagator (8) calculated in the interaction representation are [5]

$$p = 1 - \exp(-\pi\Lambda/2) = 1 - \exp\left(-\frac{\pi\Omega_0^2}{2C}\right), \tag{14a}$$

$$\phi = \frac{1}{4}\Lambda\ln\tau^2 - \frac{3}{4}\pi + \arg\Gamma\left(1 - \frac{1}{4}i\Lambda\right), \tag{14b}$$

$$\theta = 0, \tag{14c}$$

where $\tau_i = -\tau$ and $\tau_f = \tau$. Because the LZSM phase (14b) is divergent when $\tau \to \infty$, the density matrix elements (11)

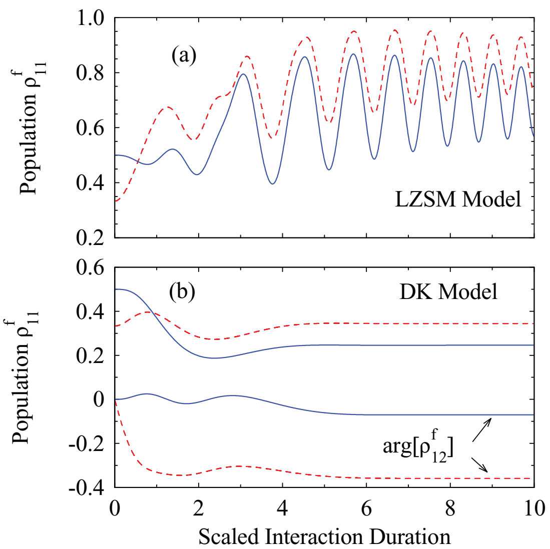

FIG. 1. (Color online) (a) Population ρ_{11}^{f} for the LZSM model vs the scaled pulse duration τ for initial superpositions $\mathbf{c}(t_{\mathrm{i}}) = [1/\sqrt{2}, 1/\sqrt{2}]^T$ (solid line) and $\mathbf{c}(t_{\mathrm{i}}) = [1/\sqrt{3}, \sqrt{2/3}]^T$ (dashed line), for $\Lambda = 2$. (b) The same for the DK model, with $\alpha = \beta = 1/2$, $\delta = 1/4$. The thin lines in this frame depict the phase of the final coherence, $\arg[\rho_{12}^{\mathrm{f}}]$

do not converge in general. In particular, for an initial pure-superposition state, the final populations oscillate and do not converge, as illustrated in Fig. 1(a) where the populations are plotted versus the interaction duration τ. Note that the oscillations are in phase, as predicted by Eqs. (11a) and (14b), which show that the oscillations phase depends on Λ and τ only, but not on the initial conditions.

In some special cases, however, the terms with the divergent phase ϕ vanish and the density matrix elements (11) are well defined. For example, one can see from Eqs. (11) that, for a completely incoherent initial state ($\rho_{12}^{\mathrm{i}} = \rho_{21}^{\mathrm{i}} = 0$), the final populations (11a) and (11c) do not contain the divergent phase ϕ. The same conclusion applies when the system starts in a single state (e.g., $\rho_{11}^{\mathrm{i}} = 1$); then $\rho_{12}^{\mathrm{i}} = 0$ and the propagator phase ϕ plays no role. The populations are well defined also in the adiabatic limit ($p = 1$) and in the diabatic limit ($p = 0$).

B. Demkov-Kunike model

1. The DK model

A powerful and flexible alternative to the LZSM model, with no divergent phases, is the DK model [3], for which the coupling and the detuning are defined by

$$\Omega(t) = \Omega_0 \mathrm{sech}(t/T), \quad \Delta(t) = \Delta_0 + B \tanh(t/T), \tag{15}$$

where Ω_0, Δ_0, B, and T are constants; we assume for simplicity that all these are nonnegative.

The Cayley-Klein parameters of the propagator for the DK model read [3]

$$a = \frac{\Gamma(\nu)\Gamma(\nu-\lambda-\mu)}{\Gamma(\nu-\lambda)\Gamma(\nu-\mu)}, \tag{16a}$$

$$b = -i\alpha 2^{2i\beta} \frac{\Gamma(1-\nu)\Gamma(\nu-\lambda-\mu)}{\Gamma(1-\lambda)\Gamma(1-\mu)}, \tag{16b}$$

where

$$\lambda = \sqrt{\alpha^2 - \beta^2} - i\beta, \tag{17a}$$

$$\mu = -\sqrt{\alpha^2 - \beta^2} - i\beta, \tag{17b}$$

$$\nu = \tfrac{1}{2} + i(\delta - \beta), \tag{17c}$$

and $\alpha = \Omega_0 T/2$, $\beta = BT/2$, and $\delta = \Delta_0 T/2$. The transition probability for the DK model reads [3]

$$p = 1 - \frac{\cosh(2\pi\delta) + \cosh(2\pi\sqrt{\beta^2 - \alpha^2})}{\cosh(2\pi\delta) + \cosh(2\pi\beta)}. \tag{18}$$

The DK model was derived originally in a little-known journal [3] in 1969, as pointed out elsewhere [6], and later rederived by other authors [7]. Three special cases of this model have their own merits. The Rosen-Zener model [8] is obtained for $B = 0$ and involves just a static detuning; it is the finest example of a soluble no-crossing two-level problem. The Allen-Eberly model [9] is obtained for $\Delta_0 = 0$ and it has no static detuning; it is the most direct, pulse-shaped alternative of the LZSM model. The Bambini-Berman model [10] is obtained for $B = \Delta$; its asymmetry produces a transition probability $p = \frac{1}{2}$ in the adiabatic limit. The DK model combines all these models and therefore adds an additional degree of freedom in each of them; for example, it supplements the level crossing in the AE model with a static detuning part, which allows one to move the level crossing with respect to the peak of the sech-shaped interaction.

2. AE model and its relation to the LZSM model

The AE model, which is defined by Eq. (15) with $\Delta_0 = 0$ and which is the one most directly related to the LZSM model, gives the following transition probability:

$$p = 1 - \frac{\cosh^2(\pi\sqrt{\beta^2 - \alpha^2})}{\cosh^2(\pi\beta)}. \tag{19}$$

Let us consider the limiting case $\beta \gg 1$, which is also written as $B \gg 1/T$. Then the chirp rate is so large that the detuning is nearly linear during the sech-shaped interaction. Moreover, the detuning rapidly reaches values that are so far away from resonance that the two-state system is decoupled from the field and the details of the interaction (pulse shape and time-dependent chirp) do not matter. Hence we can assert that, in this regime, the AE model reduces to the LZSM model. In this limit, the AE probability (19) reduces to

$$p = 1 - \exp\left(-\frac{\pi\alpha^2}{\beta}\right) = 1 - \exp\left(-\frac{\pi\Omega_0^2 T}{2B}\right). \tag{20}$$

Because for this model the chirp rate of the detuning $\Delta(t)$ at the crossing time $t = 0$ is $C = \dot{\Delta}(t=0) = B/T$, we find that, in this limit, the AE probability (20) reproduces the LZSM probability (14a) exactly. However, the AE model does not suffer from the unphysical features of the LZSM model and therefore it does not contain divergences. Moreover, the DK model adds an additional parameter Δ_0 to the AE model, which makes it also more flexible than the LZSM model.

3. Evolution of superpositions in the DK model

Because a and b in the DK model [Eqs. (16)] have definite phases, the final populations and coherences are defined for any initial state. Any output state can be calculated by using Eqs. (10) and (16). In Fig. 1(b) we demonstrate the convergence of the final population ρ_{11}^{f} as a function of the scaled interaction duration for the same initial pure superposition states, for which the LZSM model fails to converge.

C. Physical implementations

Quantum systems in a superposition state can be subjected to a level-crossing interaction in a variety of physical examples. One such example, which was already mentioned in Sec. II, is a laser-driven atomic or molecular transition. In this case, the electric field of the laser interacts with the dipole moment of the atom. Then the level crossing is created either by chirping the laser frequency or by time-dependent shift of the transition frequency (e.g., by time-dependent electric or magnetic fields [2]). We note that the lower limit of the integral $\mathcal{D}$ in Eq. (4) [i.e., $\mathcal{D}(t) = \int_0^t \Delta(t')dt'$], is important when the input state is a phase-sensitive superposition state, as in this paper. Our choice to set the lower limit to zero, which is the time of the crossing (in the LZSM model) or the maximum of the external field (in the DK model), is consistent with the chosen interaction representation in the form (1), and implies also that the interaction at the time $t = 0$ is real.

Another example wherein a superposition state can be subjected to a level-crossing interaction, is a spin-$\frac{1}{2}$ particle in a magnetic field, the basic tool in nuclear magnetic resonance (NMR). Now the interaction comes from the coupling of the magnetic moment $\boldsymbol{\mu}$ with the magnetic field $\mathbf{B}(t)$. The Hamiltonian is

$$\mathbf{H}(t) = -\gamma\frac{\hbar}{2}\begin{bmatrix} B_z(t) & B_x(t) - iB_y(t) \\ B_x(t) + iB_y(t) & -B_z(t) \end{bmatrix}, \qquad (21)$$

where γ is the gyromagnetic ratio. The level crossing comes from the variation of the z component of the magnetic field, $B_z(t)$. The LZSM model is clearly inadequate here because it requires infinitely large z component of the magnetic field at early and late times. On the contrary, the DK model does not have this problem because it assumes finite $B_z(t)$, sech-shaped $B_x(t)$, and zero $B_y(t)$. The lower limit of the integral $\mathcal{D}$ in the interaction representation now implies that the x axis is fixed by the condition that it coincides with $\mathbf{B}(t)$ at the time of the crossing, $t = 0$.

IV. EXTENSION TO MANY STATES: MAJORANA DECOMPOSITION

The conclusions for a two-state system presented above can easily be extended to multistate systems, which are reducible to one or more two-state systems, so that a two-state model can be used to describe the multistate dynamics. This can be done, for instance, by the Morris-Shore transformation for degenerate levels [11], by the Majorana decomposition for rf-driven transitions between angular-momentum states [12,13], by adiabatic elimination of weakly coupled far-off-resonant states [14,15], etc. The (in) applicability of the LZSM model to describe transitions between degenerate levels has been discussed in detail elsewhere [16].

Here we consider the rf-driven transitions between angular-momentum sublevels, which are reduced to two-state dynamics by using the Majorana decomposition [12,13]. This method can be applied whenever the Hamiltonian can be expressed as a linear combination of spin matrices. In this case the propagator of the system can be expressed in terms of the elements (the Cayley-Klein parameters) of the propagator for the corresponding two-state system (whose Hamiltonian has the same expansion coefficients in front of the spin-$\frac{1}{2}$ matrices) [13],

$$\mathbf{U}_{rs}^{(N)} = \sum_q \left[C_q^{r-1}C_q^{s-1}C_{s-1-q}^{N-r}C_{r-1-q}^{N-s}\right]^{1/2} \times a^{N+1-r-s+q}(a^*)^q b^{s-1+q}(-b^*)^{r-1+q}, \qquad (22)$$

where $C_k^n = n!/[k!(n-k)!]$ denotes the binomial coefficient and the summation over q goes over all integers for which the factorials in the Cs are defined (i.e., from $q = \max\{0, r+s-N-1\}$ to $q = \min\{r-1, s-1\}$). For $N = 2$ this propagator coincides with Eq. (7). Yet, for the LZSM model, the divergent phase ϕ in the propagator, Eq. (14b), does not allow us to start from an arbitrary superposition state, but only from a single state.

As an example we take $N = 3$. This corresponds to a Hamiltonian

$$\mathbf{H}(t) = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & \Omega(t)e^{-i\mathcal{D}(t)} & 0 \\ \Omega(t)e^{i\mathcal{D}(t)} & 0 & \Omega(t)e^{-i\mathcal{D}(t)} \\ 0 & \Omega(t)e^{i\mathcal{D}(t)} & 0 \end{bmatrix}, \qquad (23)$$

and the propagator is

$$\mathbf{U}^{(3)} = \begin{bmatrix} a^2 & \sqrt{2}ab & b^2 \\ -\sqrt{2}ab^* & |a|^2 - |b|^2 & \sqrt{2}ba^* \\ (b^*)^2 & -\sqrt{2}b^*a^* & (a^*)^2 \end{bmatrix}. \qquad (24)$$

We note that the divergent phase ϕ, which is a part of $b = e^{i\phi}\sqrt{p}$, factorizes in the propagator elements. This property is also valid for larger dimensions and allows us to have any single state as initial state. For initial superposition states, however, the outcome of an LZSM interaction is not defined. On the contrary, for the DK model the propagator elements are defined perfectly well. In Fig. 2 we plot the population ρ_{11}^{f} in the three-state system described by the Hamiltonian (23) as a function of the scaled pulse duration τ for initial superposition states. Similar behavior is seen as in the two-state case: for the LZSM model the population oscillates versus the pulse duration, while the populations in the DK model have well-defined final values.

V. DISCUSSION AND CONCLUSIONS

The LZSM model has been used very successfully in various areas across quantum physics for estimating the transition probability when a quantum system passes through a level crossing. We have shown, however, that when the quantum system is in a general superposition state before the crossing, the LZSM model cannot describe the state after the crossing because the propagator of the LZSM

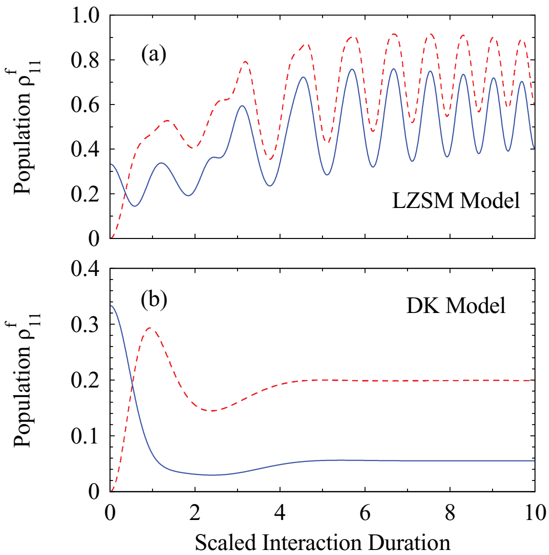

FIG. 2. (Color online) Population ρ^{f}_{11} for the three-state LZSM and DK models as a function of the scaled pulse duration τ for $\mathbf{c}(t_{\mathrm{i}}) = [1/\sqrt{3},1/\sqrt{3},1/\sqrt{3}]^T$ (solid line) and $\mathbf{c}(t_{\mathrm{i}}) = [0,1/\sqrt{2},1/\sqrt{2}]^T$ (dashed line) for (a) the LZSM model with $\Lambda = 2$ and (b) the DK model with $\alpha = \beta = 1/2$, $\delta = 1/4$.

model contains a divergent phase. This phase, which is a consequence of the unphysical assumption for an infinitely long constant interaction duration, remains hidden when the system is initially in a single quantum state or in a completely incoherent mixed state. However, for a system with nonzero initial coherence it becomes visible. We note here that it is not surprising that the unphysical nature of the LZSM model can lead to unphysical predictions; however, it is not obvious what these are. The transition probability, as is very well known, is not affected by the unphysical features of the LZSM model if the system starts from a single state; then the LZSM model allows us to predict the outcome of the interaction correctly. We have shown here that the same is true when the system starts in a completely incoherent superposition of states. However, when the initial state is a fully or partly coherent superposition of states, the LZSM is inadequate because its unphysical nature shows up in a divergent phase. In this manner we have found the rules when the LZSM model can (for a single or completely mixed initial state) or cannot (for a completely or partly coherent superposition initial state) be used.

An alternative analytically soluble level-crossing model that can be used in such cases is the DK model, which assumes a smooth bell-shaped interaction. It gives well defined propagator elements and hence convergent populations and coherences.

Similar problems are encountered in multistate systems; we have given an example with a system possessing Majorana's SU(2) dynamic symmetry. The same problem exists also there: only if we start from a single state the divergent LZ phase does not show up in the final populations. In the general case of an initial coherent superposition state the LZSM model is inadequate and one should use instead the DK model.

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