The Simplest Quantum Model Supporting the Kibble-Zurek Mechanism of Topological Defect Production: Landau-Zener Transitions from a New Perspective

Bogdan Damski

Institut für Theoretische Physik, Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany
Instytut Fizyki, Uniwersytet Jagielloński, Reymonta 4, PL-30-059 Kraków, Poland

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It can be shown that the dynamics of the Landau-Zener model can be accurately described in terms of the Kibble-Zurek theory of the topological defect production in nonequilibrium phase transitions. The simplest quantum model exhibiting the Kibble-Zurek mechanism is presented. A new intuitive description of Landau-Zener dynamics is found.

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In this Letter we present a successful combination of the Kibble-Zurek (KZ) [1,2] theory of topological defect production and quantum theory of the Landau-Zener (LZ) model [3]. Both theories play a prominent role in contemporary physics. The KZ theory predicts production of topological defects (vortices, strings) in the course of nonequilibrium phase transitions. This prediction applies to phase transitions in liquid ^{4}He and ^{3}He, liquid crystals, superconductors, ultracold atoms in optical lattices [4,5], and even to cosmological phase transitions in the early Universe [1,2]. The Landau-Zener theory has even broader applications. It has already become a standard tool in quantum optics, atomic and molecular physics, and solid state physics. The list of important physical systems governed by the LZ model grows. For instance, recent investigations point out that the smallest quantum magnets, Fe_8 clusters cooled below 0.36 K, are successfully described by the LZ model [6].

This Letter constructs the simplest quantum model whose dynamics remarkably resembles the dynamics of topological defect production in nonequilibrium second order phase transitions. The model is built on the basis of LZ theory and allows us to study the KZ mechanism of topological defect production in a truly quantum case. In addition, we present a simple, intuitive, and accurate description of LZ model dynamics.

For the rest of the Letter it is essential to introduce briefly the KZ theory. Consider a pressure quench that drives liquid ^{4}He from a normal phase to a superfluid one at a finite rate. Suppose the transition point is crossed at time $t = 0$, while time evolution starts at $t \ll 0$. As long as the liquid is far away from the transition point its time evolution is adiabatic. In other words, the relaxation time scale τ, which tells how much time the system needs to adjust to new thermodynamic conditions, is small enough. As the transition is approached the critical slowing down occurs, i.e., $\tau \to \infty$, so that at the instant $-\hat{t}$ the system leaves the adiabatic regime and enters an impulse one where its state is effectively frozen; see Fig. 1(a) for an illustration of these concepts. The time $\hat{t}$ is called the freeze-out time and was introduced by Zurek [2]. As the quench proceeds after crossing the transition point, the relaxation time scale decreases. At the instant $\hat{t}$, the system goes back into an adiabatic regime. The freeze-out time is determined by the Zurek's equation: $\tau(\hat{t}) = \hat{t}$ [2]. For the case of liquid ^{4}He, it was found experimentally that $\tau = \tau_0/|\varepsilon|$, where τ_0 is a constant, while ε is called the relative temperature. The latter measures the distance of the liquid from a transition point being at $\varepsilon = 0$, i.e., $\varepsilon(t = 0) = 0$. Physically, changes of pressure translate into changes of ε. It is further assumed that pressure changes are such that $\varepsilon = t/\tau_Q$, where τ_Q is a quench time scale. Now the Zurek's equation reads: $\tau_0\tau_Q/\hat{t} = \hat{t}$, which results in $\hat{t} = \sqrt{\tau_Q\tau_0}$. As shown in [2], knowledge of $\hat{t}$ allows for making a prediction of density of topological defects, resulting from a nonequilibrium phase transition, without solving dynamical equations describing the system.

We consider the time-dependent Hamiltonian

$$\frac{1}{2}\begin{pmatrix} \Delta t & \omega_0 \\ \omega_0 & -\Delta t \end{pmatrix} \tag{1}$$

written in the basis of time-independent states $|1\rangle$ and $|2\rangle$. Eigenstates of (1) have the form

$$\begin{bmatrix} |\uparrow(t)\rangle \\ |\downarrow(t)\rangle \end{bmatrix} = \begin{pmatrix} \cos(\theta(t)/2) & \sin(\theta(t)/2) \\ -\sin(\theta(t)/2) & \cos(\theta(t)/2) \end{pmatrix} \begin{bmatrix} |1\rangle \\ |2\rangle \end{bmatrix},$$

where $\cos(\theta) = \varepsilon/\sqrt{1+\varepsilon^2}$, $\sin(\theta) = 1/\sqrt{1+\varepsilon^2}$, $\theta \in [0, \pi]$, and $\varepsilon = \Delta t/\omega_0$. As in LZ theory $\Delta, \omega_0 > 0$ are constant parameters. The level structure of (1) is depicted in the lower part of Fig. 1, while the gap equals $\sqrt{\omega_0^2 + (\Delta t)^2}$.

Topological defects can be introduced into the LZ model in the following way. Suppose the state $|1\rangle$ corresponds to a vortex state being an eigenstate of the angular momentum operator: $\hat{L}_z|1\rangle = n|1\rangle$ ($n = \pm 1, \pm 2, \dots$), while the state $|2\rangle$ satisfies $\hat{L}_z|2\rangle = 0$. The system's wave function can be written as $|\Psi\rangle = a|1\rangle + b|2\rangle$ ($|a|^2 + |b|^2 = 1$, $\langle i|j\rangle = \delta_{ij}$). We propose to identify the density of topological defects with the average value of angular momentum

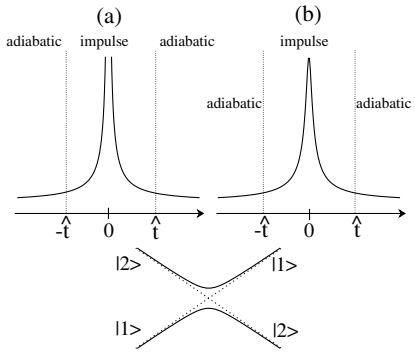

FIG. 1. Plot (a): relaxation time scale τ from the KZ theory. Plot (b): inverse of the gap in the LZ model (1). Lower plot: energy levels of the Hamiltonian (1); dotted line: $\omega_0 = 0$ case.

$\langle\Psi|\hat{L}_z|\Psi\rangle = n|a|^2$ [7]. For the rest of this discussion we define the normalized to unity density of defects as [8]

$$\mathcal{D}_n := \langle\Psi|\hat{L}_z|\Psi\rangle/n = |\langle\Psi|1\rangle|^2. \tag{2}$$

Suppose now that the system undergoes adiabatic time evolution from the ground state of (1) at $t \to -\infty$ to the ground state of (1) at $t \to \infty$. Therefore, the state of the system undergoes the ''phase transition'' from $|1\rangle$ to $|2\rangle$, i.e., from a vortex-defected ''phase'' to a vortex-free one. If the time evolution fails to be adiabatic, which is usually the case, the final state of the system is a superposition of states $|1\rangle$ and $|2\rangle$ so that the final density of the topological defects becomes nonzero. We will show that the KZ-like theory predicts surprisingly correctly vortex density (2) as a function of a transition rate only.

Analogs of the relaxation time scale, relative temperature, and quench time scale are identified as follows. First of all, let us recall the ingenious simplification of the system's dynamics in the KZ theory. The simplification relies on the assumption that the system either evolves adiabatically, i.e., adjusts perfectly to changes of parameters, or becomes immobilized, i.e., undergoes the so called impulse evolution [2]. As proposed by Zurek, the switch between adiabatic/impulse regimes is determined by the relaxation time scale, which is small during an adiabatic evolution and large in the impulse part. We would like to employ a similar strategy below. From the adiabatic theorem one knows that as long as the inverse of the gap is small enough the system starting evolution from a ground state remains in the ground state. It naturally suggests that inverse of the gap, being necessarily small in the adiabatic part of evolution, can be considered as a quantum mechanical equivalent of the relaxation time scale introduced above: we set $\tau = 1/\sqrt{\omega_0^2 + (\Delta t)^2}$ [9]. The equivalent of the relative temperature ε, i.e., a dimensionless distance of the system from anticrossing, is $\Delta t/\omega_0$. As a quench time scale τ_Q we take ω_0/Δ, while ω_0 we identify with $1/\tau_0$. Finally, we arrive at

$$\tau = \frac{\tau_0}{\sqrt{1+\varepsilon^2}}, \qquad \varepsilon = \frac{t}{\tau_Q}. \tag{3}$$

For $|\varepsilon| \gg 1$ expressions (3) are identical as those introduced above in the context of topological defect production in liquid ^{4}He, which will be commented on below.

In the following we consider dynamics of the LZ model described by the Schrödinger equation $i\frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle$, with $\hat{H}$ given by (1). We assume that time evolution starts from a ground state of (1) at some $t = t_i$ and lasts till $t_f \to +\infty$. The quantity of interest will be density of defects (2) at the end of the time evolution, which is in fact the probability of finding the system in the excited eigenstate at t_f. Adopting the KZ simplification of the system's dynamics, we assume that the evolution of the system is either adiabatic or diabatic. The adiabatic part takes place when the system is away from the anticrossing, while the diabatic part takes place in the neighborhood of an anticrossing, where the inverse of the gap is so large that the system no longer adjusts to the changes of the Hamiltonian [Fig. 1(b)]—compare to the pressure induced quench in ^{4}He described above. Therefore, the two nontrivial schemes can be considered.

(A) $t_i < -\hat{t}$: the evolution starts in the adiabatic regime, so it is adiabatic from t_i till $-\hat{t}$, then impulse from $-\hat{t}$ to $\hat{t}$, and finally adiabatic from $\hat{t}$ to t_f; see Fig. 1(b).

(B) $t_i \in [-\hat{t}, \hat{t}]$: the evolution starts in the impulse regime, therefore it is impulse from t_i to $\hat{t}$ and then adiabatic from $\hat{t}$ to t_f; compare to Fig. 1(b).

The statement that the evolution is impulse means that the system's wave function changes by the overall phase factor only. It is also assumed that we do not consider slow time evolutions for which the system stays whole time in the adiabatic regime due to the finite gap of the LZ model. Such evolutions would be incompatible with KZ considerations where divergence of the relaxation time scale at the transition point, Fig. 1(a), prohibits adiabatic evolutions close to the transition point. The assumptions standing behind the *A(B)* scheme classification are approximate and heuristic as the whole KZ theory is, and our aim is to find how good they work in the LZ system.

The only quantity that is still unknown is the instant $\hat{t}$. It is found from the equation originally proposed by Zurek in the context of classical phase transitions [2]

$$\tau(\hat{t}) = \alpha\hat{t}, \tag{4}$$

and modified by us by a factor $\alpha = \mathcal{O}(1)$, i.e., the only free parameter of our theory *independent* of τ_Q and τ_0. The solution of (4) reads

$$\hat{\varepsilon} = \varepsilon(\hat{t}) = \frac{1}{\sqrt{2}}\sqrt{\sqrt{1+\frac{4}{x_\alpha^2}} - 1}, \qquad x_\alpha = \alpha\frac{\tau_Q}{\tau_0}. \tag{5}$$

The first observation shows that for fast transitions, i.e., $x_\alpha \to 0$ at τ_0 being fixed, one gets $\hat{t} = \sqrt{\tau_0\tau_Q/\alpha}$.

Therefore,we recover, up to $\mathcal{O}(1)$ factor, the well known result [2]. It happens because in the fast transition limit $\hat{\varepsilon} \gg 1$ and then $\tau(\hat{\varepsilon}) \approx \tau_0/\hat{\varepsilon}$, which is the same as in the theory of dynamics of quantum phase transitions in liquid ^{4}He [2]. This observation further supports similarities of our model to KZ systems.

For the first application of our theory we consider the situation when time evolution starts far away from the anticrossing—a generic A scheme case. Taking $|\Psi(t_i)\rangle = |\downarrow(t_i)\rangle$ as an initial system's wave function, and assuming limits $t_i \to -\infty$ and $t_f \to \infty$, one easily gets the following final density of topological defects,

$$\mathcal{D}_n = |\langle\Psi(t_f)|1\rangle|^2 \approx |\langle\uparrow(\hat{t})|\downarrow(-\hat{t})\rangle|^2 = \frac{\hat{\varepsilon}^2}{1+\hat{\varepsilon}^2}. \quad (6)$$

A derivation of (6) uses the following relations: $|\langle\uparrow(t_f)|\Psi(t_f)\rangle| \approx |\langle\uparrow(\hat{t})|\Psi(\hat{t})\rangle| \approx |\langle\uparrow(\hat{t})|\Psi(-\hat{t})\rangle| \approx |\langle\uparrow(\hat{t})|\downarrow(-\hat{t})\rangle|$. Substitution of (5) into (6) gives

$$\mathcal{D}_n = \frac{2}{\mathcal{P}(x_\alpha)}, \qquad \mathcal{P}(x_\alpha) = x_\alpha^2 + x_\alpha\sqrt{x_\alpha^2+4} + 2. \quad (7)$$

Expanding $\mathcal{D}_n$ into a series one gets for fast transitions

$$\mathcal{D}_n = \exp(-x_\alpha) + \mathcal{O}(x_\alpha^3), \quad (8)$$

which is an exact result up to $\mathcal{O}(x_\alpha^3)$ terms if the constant α is chosen as $\pi/2$ [3]. Notice that $\alpha = \mathcal{O}(1)$ as assumed in (4). In the adiabatic limit ($x_\alpha \to \infty$), Eq. (7) predicts $\mathcal{D}_n = \mathcal{O}(1/x_\alpha^2)$ instead of exponential decay, which does not affect results much due to the very small value of $\mathcal{D}_n$ in that regime.

The best performance for fast transitions can be understood as follows. The derivation of (6) requires the assumption that in the time interval $[-\hat{t}, \hat{t}]$ the state of the system does not change essentially. The smaller this time interval is, the better is this assumption. From (3) and (5) one easily finds that $\hat{t}/\tau_0$ grows monotonically with x_α. Indeed, $\hat{t}/\tau_0$ equals $\sqrt{x_\alpha}/\alpha$ for $x_\alpha \to 0$ and increases to $1/\alpha$ for $x_\alpha \to \infty$. Therefore it is not surprising that our predictions work better for fast transitions.

Now we would like to discuss the situation when time evolution starts from a ground state at the anticrossing center, $t_i = 0$, which is a generic B scheme situation. As $t_f \to \infty$ one gets

$$\mathcal{D}_n = |\langle\uparrow(\hat{t})|\downarrow(0)\rangle|^2 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{1+\hat{\varepsilon}^2}}\right), \quad (9)$$

where we put $|\Psi(0)\rangle = |\downarrow(0)\rangle = -\frac{\sqrt{2}}{2}|1\rangle + \frac{\sqrt{2}}{2}|2\rangle$, and assumed that $|\langle\uparrow(t_f)|\Psi(t_f)\rangle| \approx |\langle\uparrow(\hat{t})|\Psi(\hat{t})\rangle| \approx |\langle\uparrow(\hat{t})|\Psi(0)\rangle|$. Combining (5) and (9) one gets

$$\mathcal{D}_n = \frac{1}{2}(1 - \sqrt{1 - 2/\mathcal{P}(x_\alpha)}), \quad (10)$$

with x_α and $\mathcal{P}(x_\alpha)$ defined in (5) and (7). The agreement of this expression with the results of numerical calculations is remarkable as depicted in Fig. 2. It is even better than in the previous case when we considered the evolution starting far away from the avoided crossing. We attribute it to the fact that now the frozen part takes less time, i.e., $\hat{t}$ instead of $2\hat{t}$, and to the absence of the approximation that the initial stage of evolution is adiabatic.

We can also easily calculate the density of defects when time evolution starts in the impulse regime (B scheme), but outside the avoided crossing center. Taking $|\Psi(t_i)\rangle = |\downarrow(t_i)\rangle := -\sin(\theta_0/2)|1\rangle + \cos(\theta_0/2)|2\rangle$ we obtained

$$\mathcal{D}_n = -\frac{\cos(\theta_0)}{\sqrt{2\mathcal{P}(x_\alpha)}} + \frac{1 - \sqrt{1 - 2/\mathcal{P}(x_\alpha)}\,\sin(\theta_0)}{2}, \quad (11)$$

where $\theta_0 = \arctan((\omega_0/(\Delta t_i)) \in [0, \pi]$ measures the distance of the starting point of time evolution from an avoided crossing, e.g., $\theta_0 = \pi/2$ when evolution starts from an anticrossing center and then Eqs. (10) and (11), are identical.

A comparison of (11) to numerics for $\tau_Q/\tau_0 \leq 1.75$ and $|\theta_0 - \pi/2| \leq \pi/10$ reveals satisfactory agreement; see Fig. 3 for a typical situation. For larger τ_Q/τ_0 and/or $|\theta_0 - \pi/2|$ the agreement gradually decreases, which we attribute to the fact that for these parameters the starting time moment, $t_i = \tau_Q/\tan\theta_0$, might be outside $[-\hat{t}, \hat{t}]$, so that the assumption that the initial stage of time evolution is impulse can be wrong. One avoids these problems when either $t_i \ll -\hat{t}$ or $|t_i| \ll \hat{t}$, i.e., when the system evolves clearly within the A or B scheme, respectively.

Having at hand the above obtained results, let us comment on the Zurek-like equality (4) extensively used in this Letter. This equality gives the time moments $\pm\hat{t}(\tau_Q)$, which separate the adiabatic and impulse regimes [10]. Do we need to rely on this equation? To answer this question we notice that we aim at getting the best description of LZ model dynamics by using the simplification that the evolution is either adiabatic or impulse in the sense specified below the *A(B)* scheme description. It means that the whole problem can be reduced to getting the time

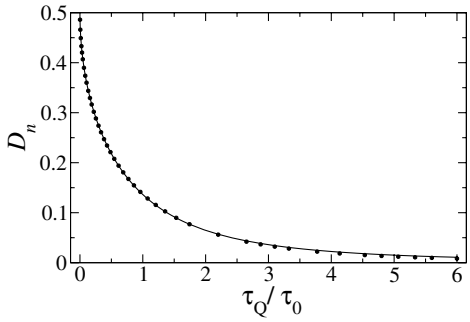

FIG. 2. Density of defects for the system whose evolution starts at the anticrossing center. Solid line—prediction (10), dots—numerical data. The parameter $\alpha = 0.77$ was found from a fit of (10) to numerics.

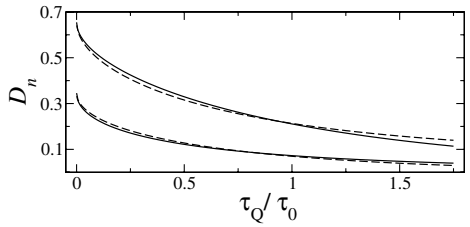

FIG. 3. Density of defects. Solid lines—numerics, dashed lines—Eq. (11) with α determined from the fit. Upper (lower) curves correspond to $\theta_0 = 0.6\pi$, $\alpha = 1.06$ ($\theta_0 = 0.4\pi$, $\alpha = 0.58$).

moments $\pm\hat{t}$ that lead to the best comparison of the defect density to exact results. This can be done without Eq. (4) by fitting the $\hat{t}(\tau_Q)$ directly to numerical/analytical data. Equation (4) reduces the problem of getting optimal $\hat{t}(\tau_Q)$ to fitting just one parameter, α, instead of fitting a whole function $\hat{t}(\tau_Q)$. Naturally, it is of fundamental interest to try to find analytically the best $\hat{t}(\tau_Q)$ function and compare it to that taken directly from the KZ theory.

Let us point out the possible usefulness of these considerations in the understanding of nonequilibrium quantum phase transitions (QPTs). There is no doubt that quantum many-body systems of interest (spin systems, cold atoms in optical lattices) are more complicated than the LZ model. It is, however, generally accepted that close to the generic second order QPT point there exists an anticrossing between a ground state and a first excited state—see Chap. 1.1 of [11] and Sec. 2.4 of [12]. Therefore, one can expect that at least a qualitative picture of the change of the system's properties during a QPT can be captured by a simple two level model, e.g., the LZ model. If another sort of a two level approximation would work better, it is still likely that the same analysis as the one presented here would work. Once the many-body model of interest is specified and its low energy static properties are determined, one can define an equivalent of the ''density of defects'' and study the system's dynamics using the tools presented in this Letter.

Let us look at other possible extensions of this work. First of all, it is desired to reanalyze more strictly the LZ dynamics to get a systematic control of the intuitive results obtained above. This work can be done utilizing the results from [13]. Second, it seems to be very interesting to investigate how the adiabatic/impulse simplification of system dynamics works in other quantum mechanical systems, for instance those which exhibit a faster increase of the gap with the distance from anticrossing. We expect to get better qualitative agreement in these cases.

Several other remarks are in order. First of all, we have shown that the very simple LZ model successfully reproduces KZ-like dependence of topological defect density on the quench rate. Second, our results provide an intuitive description of LZ model dynamics unexplored up to now in numerous papers devoted to the LZ model. Notice that with our intuitive approach we have been able to obtain qualitatively correct predictions concerning LZ model dynamics *without* solving the time-dependent Schrödinger equation. Third, we show that the KZ theory can provide predictions beyond the lowest nontrivial τ_Q/τ_0 order usually considered [2,5,14]. Fourth, our results are directly applicable to different quantum two level systems, e.g., to the molecular magnets Fe_8 [6].

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[8] Considering the freedom in choosing the states $|1\rangle$, $|2\rangle$, it is clear that other, nonvortex based definitions of defect densities can be worked out when a particular form of wave functions is assumed.
[9] Other definitions of τ seem to be equally plausible on the heuristic level considered here, e.g., $\tau = \omega_0/[\omega_0^2 + (\Delta \cdot t)^2] \sim 1/\mathrm{gap}^2$. We studied a few such choices of τ and found that the simplest one, $\tau \sim 1/\mathrm{gap}$ discussed in the Letter, compares the best to exact results.
[10] Notice that $\hat{t}(\tau_Q)$ provides Zurek's freeze-out time for different transitions labeled by τ_Q, but all of them starting from the same initial (ground) state, e.g., from the ground state at the center of the anticrossing.
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